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Key Points:

- We review the key questions surrounding isoGDGT-based proxies in the marine environment and highlight future research priorities
- IsoGDGTs are primarily sourced from Marine Group I Nitrososphaeria and exported predominantly from the 0–250 m depth range
- Temperature exerts a first-order control on isoGDGT cyclization but the TEX₈₆-SST response beyond the modern range (>30°C) is uncertain

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Archaeal Tetraether Lipids as Tracers for Past Marine Environmental Change

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Abstract Archaea are single-celled microorganisms that are abundant in marine environments and play a key role in the carbon and nitrogen cycles. Archaea can biosynthesize a wide variety of isoprenoid membrane lipids, including isoprenoid glycerol dibiphytanyl glycerol tetraethers (isoGDGTs). Experimental and empirical evidence demonstrates that the number of cyclopentane moieties in isoGDGTs is related to growth temperature, leading to the formulation and development of the TEX₈₆ ocean temperature proxy. The TEX₈₆ proxy has been widely applied to marine sediments spanning the last 190 million years and has revealed unique insights into the evolution of ocean temperatures over diverse timescales. Other indices have been developed using archaeal lipids to reconstruct ecological and biogeochemical processes that operate within the marine realm. However, several knowledge gaps (e.g., depth of export production, non-temperature controls, application in non-

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analogue climates) limit the application of archaeal lipid-based proxies in modern and ancient marine environments. In this review, we critically assess the utility of archaeal lipids as tracers for (paleo) environmental change, with an emphasis on the TEX₈₆ paleotemperature proxy.

Plain Language Summary Archaea are single-celled microbes that thrive in the ocean. The cell's outer layer consists of a lipid membrane. Archaea modify the molecular composition of their lipid membranes in response to changing environmental conditions, notably the temperature of the seawater in which they grow. This led scientists to express the distribution of these lipids as a ratio (TEX₈₆) which is calibrated with temperature through studies of modern ocean sediments. These calibration equations can be used to reconstruct past ocean temperatures. Archaeal lipids have also helped scientists understand other environmental and ecological changes in past marine environments. However, many questions about the application of archaeal lipid-based ratios in marine environments remain unanswered. For example, where are these lipids produced in the ocean? Is temperature the only control on the TEX₈₆ ratio? Can we apply calibration equations based on modern climate to all past climate states? This review examines the utility of archaeal lipids for reconstructing environmental change in the ocean and suggests directions for future research.

1. Introduction

Following their recognition as a separate domain of life in the late 1970s (Woese & Fox, 1977), archaea were thought to be confined to (hyper)thermophilic and hypersaline environments (Woese et al., 1978). However, nearly two decades later archaea were found to be ubiquitous in mesophilic marine environments (e.g., DeLong, 1992; Fuhrman et al., 1992) and have subsequently been identified in a diverse range of non-marine environments (e.g., mineral soils, peat, lakes; for reviews see Baker et al., 2020; Schleper et al., 2005). Archaea biosynthesize unique glycerol ether membrane lipids that are composed of isoprenoid alkyl chains connected by ether bonds to one or two terminal glycerol moieties (De Rosa & Gambacorta, 1988; Koga & Morii, 2005). These exist as intact polar lipids (IPLs) consisting of a polar headgroup connected to a core lipid (Gambacorta et al., 1995) in living cells or as core lipids after cell lysis and degradation (e.g., Harvey et al., 1986; Lengger et al., 2012). There are two main core lipid structures: (a) isoprenoid glycerol diphytanyl diethers (comprising two phytanyl, i.e., C₂₀, chains linked to a single glycerol unit) and (b) isoprenoid glycerol dibiphytanyl glycerol tetraethers (comprising two biphytanyl, i.e., C₄₀, chains linked to two glycerol units; isoGDGTs). In marine sediments, isoGDGTs are typically much more abundant than archaeal diether lipids (Hingley et al., 2024; Lipp & Hinrichs, 2009; Liu et al., 2012a). Multiple groups of planktonic archaea have been proposed to contribute isoGDGTs to the sedimentary isoGDGT pool (e.g., Lincoln et al., 2014b, 2014a; Ma et al., 2020; Schouten et al., 2000, 2014; Turich et al., 2007). However, isoGDGTs in marine sediments are now thought to dominantly derive from planktonic ammonia-oxidizing archaea (Zeng et al., 2019, 2022), which are taxonomically affiliated with the class *Nitrososphaeria* within the phylum *Thermoproteota* (Oren & Garrity, 2021; Rinke et al., 2021), and were previously called Thaumarchaeota (Brochier-Armanet et al., 2008) or marine Crenarchaeota (DeLong, 1992; Fuhrman et al., 1992).

IsoGDGTs can contain up to eight cyclopentane moieties (e.g., De Rosa, De Rosa, Gambacorta, Minale, & Bu'Lock, 1977) and early studies demonstrated that the number of cyclopentane moieties in isoGDGTs increased with growth temperature in thermophilic archaeal cultures (e.g., De Rosa, Esposito, et al., 1980; Trincone et al., 1989). This relationship has been expressed using the ring index (RI; Pearson et al., 2004), which is the weighted average of cyclopentane or cyclohexane moieties, where “isoGDGT-X” is an isoGDGT with X cyclopentane moieties (note that variations to this formula are used in the literature):

$$RI = \frac{[\text{isoGDGT} - 1] + 2 \times [\text{isoGDGT} - 2] + 3 \times [\text{isoGDGT} - 3] + \dots n \times [\text{isoGDGT} - n]}{[\text{isoGDGT} - 0] + [\text{isoGDGT} - 1] + [\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + \dots [\text{isoGDGT} - n]} \quad (1)$$

In marine mesophilic environments, isoGDGTs contain up to four cyclopentane moieties. Sinninghe Damsté et al. (2002) identified an isoGDGT with a unique structure of four cyclopentane moieties and one cyclohexane moiety (crenarchaeol). Sinninghe Damsté et al. (2002) also identified an isomer of crenarchaeol which possibly represents a biological adaptation to higher temperatures (e.g., Bale, Palatinszky, et al., 2019; Sinninghe Damsté et al., 2018). Schouten et al. (2002) observed that the number of cyclopentane moieties for isoGDGTs preserved in

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marine surface sediments increased with increasing sea surface temperature (SST). This was expressed in a ratio, the TetraEther indeX of tetraethers consisting of 86 carbons (TEX₈₆):

$$\text{TEX}_{86} = \frac{[\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol isomer}]}{[\text{isoGDGT} - 1] + [\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol isomer}]} \quad (2)$$

TEX₈₆ values of a set of globally distributed marine surface sediments were highly correlated with SST and, to a lesser extent, shallow subsurface temperature (i.e., 100 m), which was explained by the notion that these sedimentary isoGDGTs were derived predominantly from archaea thriving in (sub)surface waters of the ocean (Schouten et al., 2002). The abundant isoGDGT-0 and crenarchaeol were excluded from TEX₈₆ as they mask the temperature-dependent variability of the minor isoGDGTs (i.e., isoGDGT-1 to isoGDGT-3). IsoGDGT-0 was also excluded because it can be derived from multiple archaeal sources that do not necessarily respond to temperature in the same way as *Nitrososphaeria*, such as sedimentary methanogenic archaea (Schouten et al., 2002).

TEX₈₆ captures millennial-scale SST changes during the Last Glacial Maximum (29,000–19,000 years ago; Hugué et al., 2006c), glacial-interglacial SST changes during the Quaternary (2.58 million years ago (Ma) to now) and Pliocene (5.3–2.6 Ma; Hugué et al., 2011; Lopes dos Santos et al., 2013; Thomas et al., 2014), and astronomical-scale SST changes during the Pliocene and beyond (Fokkema, Brinkhuis, et al., 2024; Lawrence et al., 2020). These and many other studies have demonstrated that TEX₈₆-based SSTs have a strong coherence with SSTs derived from other organic (e.g., the alkenone U^{K'}₃₇ proxy; e.g., Lawrence et al., 2020; Lopes dos Santos et al., 2013; Naafs et al., 2020) and inorganic paleothermometers (e.g., Mg/Ca; Crouch et al., 2020; Zachos et al., 2006)—this observation is found within different oceanic basins and across different timescales. TEX₈₆ is particularly useful when other temperature proxies cannot be applied, such as in carbonate-poor marine sediments lacking planktonic foraminifera (e.g., Jenkyns et al., 2012; Sluijs et al., 2006), when alkenones are absent (e.g., Petrick et al., 2023; Zhang et al., 2014), or when temperatures exceed the alkenone-based U^{K'}₃₇ paleothermometer upper limit of 29°C (Müller et al., 1998; Pahl et al., 1988). A recent ~485-million-year reconstruction of Earth's surface temperature (Judd et al., 2024) demonstrates that TEX₈₆ plays a key role in reconstructing ocean temperatures over the past 190 million years (Figure 1), especially during the Mesozoic (~190–66 Ma) and Paleogene (~66–23 Ma) where there are fewer methods available to reliably reconstruct SST (e.g., Auderset et al., 2020; Forster et al., 2007; Inglis et al., 2015a; Jenkyns et al., 2004; O'Brien et al., 2017; Robinson et al., 2017; Schouten et al., 2003b). For example, TEX₈₆-based temperature estimates revealing tropical SSTs >30°C during past greenhouse climates have helped refute the “tropical thermostat” hypothesis (Forster et al., 2007; Pearson et al., 2007; Schouten et al., 2003b). It has also been an indispensable proxy in the high-latitudes where there are fewer methods available to estimate SST (see Hollis et al., 2019 and ref. therein) and revealed that the pole-to-equator temperature gradient was reduced during past episodes of warm climate states (e.g., Jenkyns et al., 2004; Sluijs et al., 2006).

Applications of TEX₈₆ now span from the Early Jurassic (i.e., 190 Ma) to present and thousands of data points have been added to publicly available repositories since 2002 (Figure 1; Judd et al., 2022). Yet, despite its widespread application in marine paleo-environments, various questions remain. Firstly, the TEX₈₆ proxy implies that isoGDGTs in marine sediments are derived from a single group of archaea (*Nitrososphaeria*) living in the upper ocean. While this is supported by the similarity between isoGDGT distributions in surface sediments and those in *Nitrososphaeria* cultures (Sinninghe Damsté et al., 2002) molecular evidence shows that *Nitrososphaeria* occur throughout the water column (e.g., Karner et al., 2001; Schattenhofer et al., 2011; Teira et al., 2006). This implies that the sedimentary isoGDGT pool may include contributions from non-surface dwelling *Nitrososphaeria* living in the subsurface and/or deep ocean (e.g., Ho & Laepple, 2016; Kim et al., 2012a; Schouten et al., 2002; Taylor et al., 2013; Tierney & Tingley, 2015; van der Weijst et al., 2022), although the exact contribution remains debated. Secondly, the membrane lipid composition of *Nitrososphaeria* may be influenced by various other ecological and physiological factors besides temperature (e.g., nutrient availability and community composition; Elling et al., 2015; Hurley et al., 2016; Qin et al., 2015; Rattanasriampaipong et al., 2025). Thirdly, the TEX₈₆-SST relationship from globally-distributed marine surface sediments carries uncertainties at both temperature extremes. At low temperatures (<~15°C), the relationship shows poor temperature sensitivity (i.e., polar regions; Fietz et al., 2016, 2020; Ho et al., 2014; Kim et al., 2010, 2012a; Seki et al., 2014). At high temperatures (>~30°C), it requires extrapolating the TEX₈₆-temperature relationship beyond the modern calibration range. Various attempts to extend the TEX₈₆-temperature relationship >30°C have been made

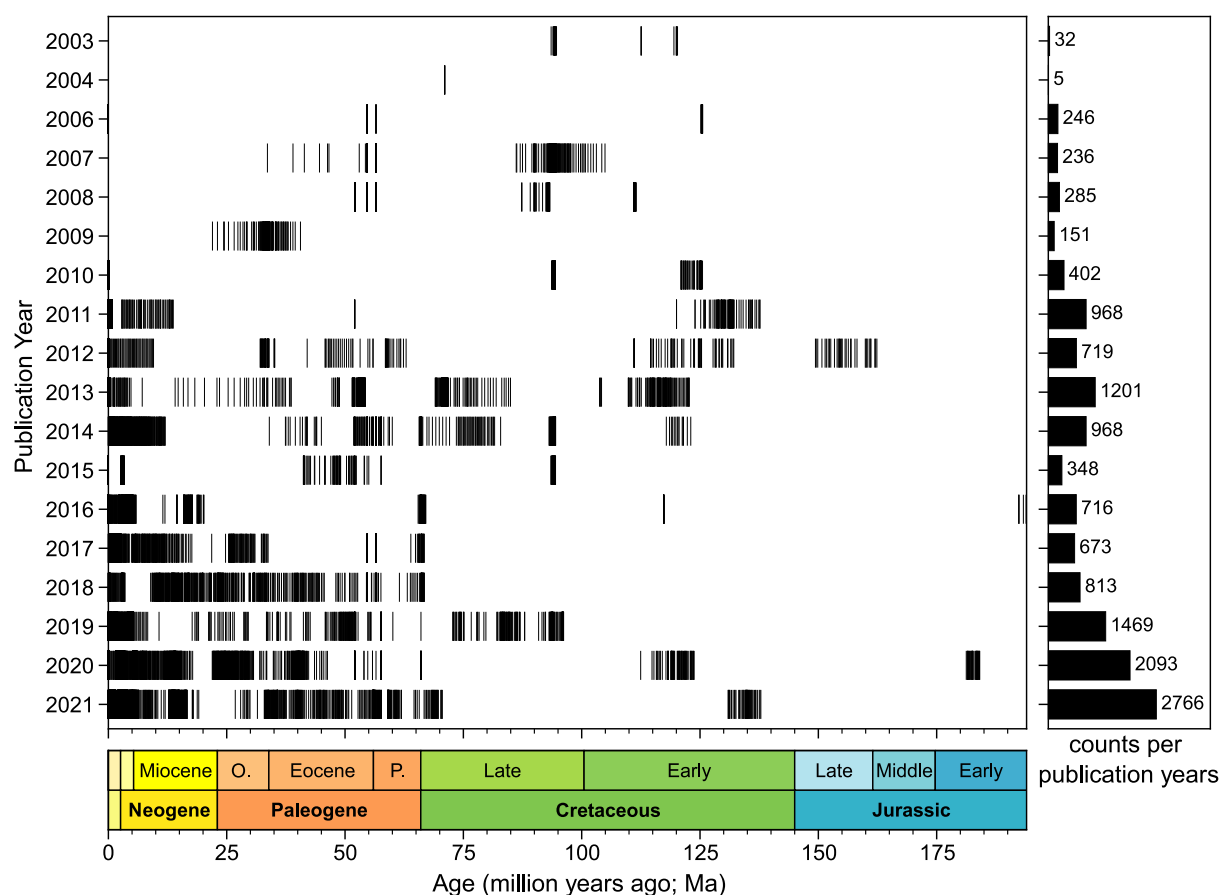


Figure 1. TEX_{86} paleotemperature data cover most of geological time since the Jurassic. The panel on the left shows the temporal coverage of TEX_{86} data sets published in each year between its first application in 2003 and 2021. Some data sets were updated since their first publication and appear in their most recent publication in this figure. The panel on the right shows the number of TEX_{86} data points published each year. Compiled from the PhanSST database (Judd et al., 2022).

(e.g., O'Brien et al., 2017; Schouten et al., 2007b; Tierney & Tingley, 2014). However, the mathematical relationship between TEX_{86} and $\text{SST} > 30^{\circ}\text{C}$ (i.e., linear vs. exponential) is unclear and different calibrations lead to markedly different reconstructed temperatures, especially during greenhouse periods (Inglis & Tierney, 2020).

In 2023, the 2nd International workshop on GDGTs was held at ETH (Zurich, Switzerland) to discuss the steps forward in proxy understanding, development and application. As an outcome of this workshop, Bijl et al. (2025) recently summarised the best practices for *generating* GDGT data. In this review, we critically assess the *utility* of isoGDGTs as tracers for marine environmental change, with an emphasis on the TEX_{86} proxy. We describe the structural diversity, biosynthesis, and biological source(s) of archaeal membrane lipids in marine settings (Sections 2–4). We then outline the fundamental principles that underpin the TEX_{86} SST proxy (Section 5) and summarize potential confounding factors (e.g., seasonality, export production, non-thermal controls; Sections 6–8) and diagenesis (Section 9). We also highlight the role that archaeal lipids can play in studying aspects other than temperature (e.g., archaeal ecology, the deep biosphere, carbon cycling; Section 10). We conclude by identifying key knowledge gaps in archaeal lipid research and provide recommendations moving forward (Sections 11 and 12).

2. Structural Diversity of Archaeal Membrane Lipids

Numerous archaeal membrane lipids have been identified in archaeal cultures and marine environments (Figure 2). Below, we summarize the structural diversity and source of archaeal lipids (tetraethers and diethers). For the extraction and analysis of archaeal core lipids and IPLs, commonly used methods are described in Schouten et al. (2007a, 2013a), Huguet et al. (2006a, 2010), Becker et al. (2013), Hopmans et al. (2016), Wörmer et al. (2013, 2015), Zhu et al. (2013), and references cited therein.

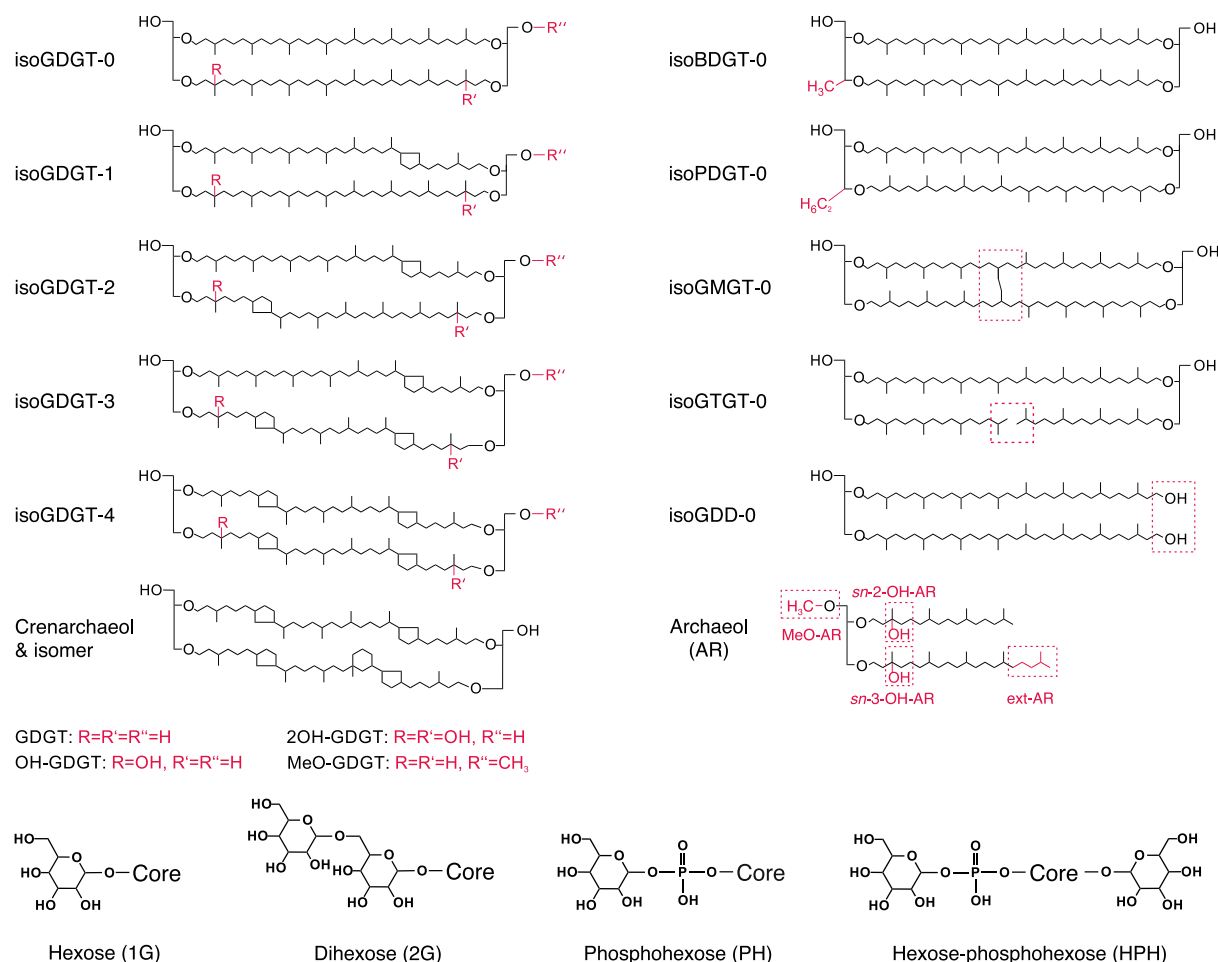


Figure 2. Structures of archaeal lipids commonly found in marine environments. The most common archaeal core lipids are isoprenoid glycerol dibiphytanyl glycerol tetraethers (isoGDGT) and glycerol diphytanyl diethers (archaeol, AR). Archaeol derivatives may contain one or two extended sidechains (ext-AR and 2ext-AR), one or two additional hydroxyl groups at different positions (*sn*-2-OH-AR, *sn*-3-OH-AR, or 2-OH-AR), or a methoxy group at the *sn*-1 position of the glycerol moiety (MeO-AR). IsoGDGTs may contain up to four cyclopentane moieties (isoGDGT-0 to -4) or one cyclohexane and four cyclopentane moieties (crenarchaeol and its isomer). IsoGDGTs may also contain one (OH-isoGDGT) or two (2OH-isoGDGT) additional hydroxyl groups and zero to four cyclopentane moieties in the biphytanyl side chain (OH-isoGDGT-0 to -4). Other derivatives are isoprenoid glycerol monoalkyl glycerol tetraethers (isoGMGTs), isoprenoid glycerol dibiphytanyl glycerol tetraethers (isoPDGTs) as well as isoGDGTs containing a methoxy group at the *sn*-1 position of the glycerol moiety (MeO-isoGDGT). Isoprenoid glycerol trialkyl glycerol tetraethers (isoGTGTs) likely are biosynthetic intermediates or side products. Archaeal intact polar lipids consist of one or two glycosidic or glycoposphatidic headgroups attached to the glycerol *sn*-1 hydroxyl position of an archaeol or isoGDGT core lipid. Only some representative headgroups are shown (i.e., hexose, dihexose, phosphohexose and hexose-phosphohexose), and headgroup structural diversity in the environment may be higher. Structural assignments such as glycerol configuration, ring position, position of hydroxyl groups in the biphytanyl moieties of isoGDGTs, and the crosslink between biphytane chains in isoGMGTs have been determined only for some of the displayed compounds (De Rosa, Gambacorta, et al., 1980; Ferrante et al., 1988; Galliker et al., 1998; Gräther & Arigoni, 1995; Holzheimer et al., 2021; Langworthy, 1977; Liu et al., 2012c; Morii et al., 1998; Sinninghe Damsté et al., 2002).

2.1. Frequently Occurring Tetraether Lipids

Although archaeal lipids like archaeol have been known since the early 1960s (Kates et al., 1963; Sehgal et al., 1962), the first reports of isoGDGTs, discovered in cultures of extremophilic archaea, date back to the 1970s (Chappe et al., 1979; De Rosa, De Rosa, Gambacorta, Minale, & Bu'Lock, 1977; De Rosa & Gambacorta, 1988; Heathcock et al., 1985; Langworthy, 1977; Langworthy et al., 1982). IsoGDGTs possess zero to eight cyclopentane moieties (Figure 2), but isoGDGT-5 to isoGDGT-8 are absent in non-hydrothermally influenced marine sediments (Schouten et al., 2013b, and references therein). There are also various minor isomers associated with isoGDGT-1 to isoGDGT-4 and crenarchaeol (Becker et al., 2013; Elling et al., 2017; Hopmans et al., 2016; Sinninghe Damsté et al., 2002). Becker et al. (2013) and Hopmans et al. (2016) speculated that these minor isomers may represent either regioisomers or structural isomers, which is supported by the observation that the

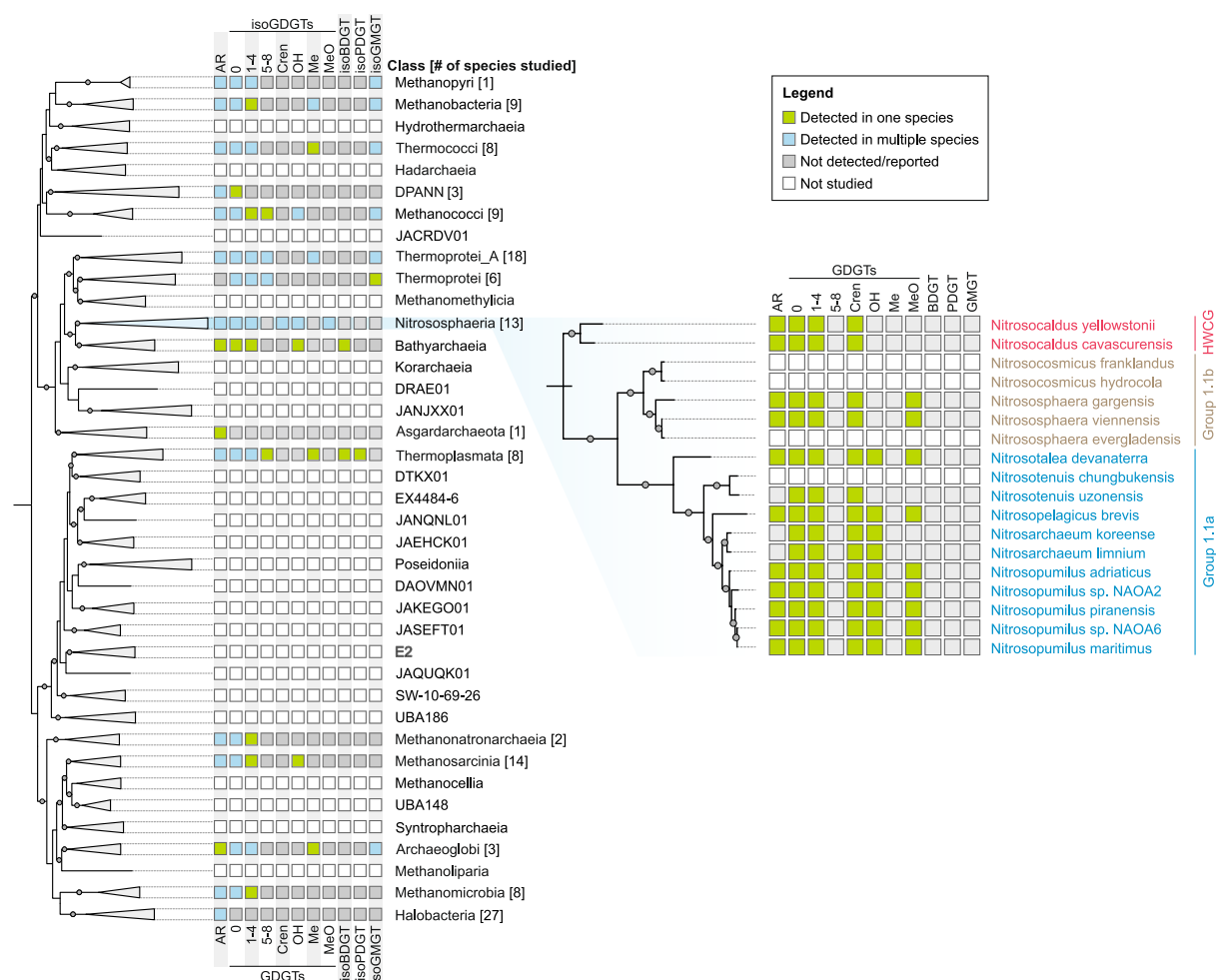


Figure 3. Occurrence of membrane lipid types among archaea. The panel on the left shows the occurrence of lipid types among archaea clustered at the class level next to a phylogenomic tree (concatenated proteins, see below; DPANN and Asgardarchaeota clustered at superphylum/phylum level). The inset shows the occurrence of lipid types in *Nitrososphaeria* (next to a 16S rRNA gene phylogenetic tree), the dominant source of isoGDGTs to marine mesophilic sediments. Occurrence was indicated as “detected” when the lipid type was detected in at least one cultivated representative of the class/phylum. Lipid occurrence data was compiled from 70 studies using different extraction and analysis methods and covering 131 strains (Elling et al., 2026). The phylogenomic tree is based on 695 archaeal genomes, with one representative genome per family of archaea randomly picked from the Genome Taxonomy Database (Parks et al., 2022), plus all available genomes from species with studied lipid composition. Marker proteins were identified, concatenated, and aligned using GTDB-Tk (v2.2.5 with reference data version r207; Chaumeil et al., 2022) and the tree was calculated using IQTREE v2.2.0.3 (Nguyen et al., 2015). The phylogenetic tree of *Nitrososphaeria* is based on full-length or near full-length 16S rRNA gene sequences, aligned using MAFFT v7.388 (Katoh & Standley, 2013) and the tree was calculated as described above. *Nitrosotalea devanaterre* is shown as belonging to Group I.1a, as a simplification of the status of the SAGMGC1 group adjacent to Group I.1a. Circles show $\geq 90\%$ ultrafast bootstrap support for 1000 replicates. Abbreviations: AR, archaeol; 0, isoGDGT-0; 1–4, isoGDGT-1 through isoGDGT-4; 5–8, isoGDGT-5 through isoGDGT-8; Cren, crenarchaeol and isomer; OH, hydroxy isoGDGT; Me, methylated isoGDGT; MeO, methoxy isoGDGT; isoBDGT, butanetriol dibiphytanyl glycerol tetraether; isoPDGT, pentanetriol dibiphytanyl glycerol tetraether; isoGMGT, glycerol monoalkyl glycerol tetraether.

isomers do not simply represent different combinations of biphytanes (Keller et al., 2025a). IsoGDGTs are widespread among cultivated archaea, but only a subset of these produce isoGDGTs with cyclopentane moieties (Figure 3). In contrast, crenarchaeol is a unique isoGDGT because it possesses a cyclohexane moiety in addition to four cyclopentane moieties (Sinninghe Damsté et al., 2002). After this initial structural characterization, the assignment of one of its 23 chiral centers has recently been adjusted based on its total synthesis (Holzheimer et al., 2021). It was originally identified in *Cenarchaeum symbiosum*, a sponge-symbiotic marine archaeon belonging to the class *Nitrososphaeria* (Sinninghe Damsté et al., 2002) and is now considered as a specific biomarker for this class (Figure 3). Crenarchaeol has two major isomers, which were recently characterized as stereoisomers rather than regioisomers as previously thought (Liu et al., 2018; Sinninghe Damsté et al., 2018).

Lipp and Hinrichs (2009) and Liu et al. (2012c) identified isoGDGTs with one to two additional hydroxyl groups on tertiary carbon atoms (Figure 2). These hydroxylated isoGDGTs (OH-isoGDGTs) commonly contain up to four cyclopentane moieties (Elling et al., 2017; Kurth et al., 2019; Liu et al., 2012c; Sollai et al., 2019a) and rarely four cyclopentane moieties and one cyclohexane moiety (Zhang et al., 2023). Like isoGDGTs, OH-isoGDGTs are abundant in sediments from the open ocean (Huguet et al., 2013; Varma et al., 2024b) and brackish marginal seas (e.g., the Baltic Sea; Kaiser & Arz, 2016; Sinninghe Damsté et al., 2022), where they comprise up to ~20% of the combined isoGDGT and OH-isoGDGT pool (Fietz et al., 2013, 2016; Huguet et al., 2013; Kaiser & Arz, 2016; Sinninghe Damsté et al., 2022). In cultures, OH-isoGDGTs have been found in a small subset of archaea, including all mesophilic group I.1a *Nitrososphaeria* (Bale, Palatinszky, et al., 2019; Elling et al., 2017; Varma et al., 2024a) as well as a thermophilic methanogen from the class *Methanococci* (Liu et al., 2012c) and a freshwater methanotroph from the class *Methanosarcinia* (Figure 3; Kurth et al., 2019). The elevated abundance of OH-GDGT-0 in marine methane seeps further suggests that other, potentially methanotrophic, archaea may produce OH-GDGTs (Guan et al., 2024).

2.2. Infrequently Occurring Tetraether Lipids

In addition to the aforementioned tetraether lipids (isoGDGTs, OH-isoGDGTs), a wide range of other archaeal tetraether lipids are found in marine settings (Figure 2). These tetraethers are modified either in their side chain or glycerol moieties. Isoprenoid glycerol monoglycerol tetraethers (isoGMGTs), previously known as “H-shaped” isoGDGTs, have an additional covalent bond between both biphytanyl moieties (Figure 2; Morii et al., 1998). These molecules were originally thought to represent an adaptation to (hyper)thermophilic conditions (Baumann et al., 2018; Jaeschke et al., 2012; Pan et al., 2016; Sollich et al., 2017; Tourte et al., 2022; Umoh et al., 2020). However, isoGMGTs are also abundant in mesophilic marine and estuarine sediments lacking hydrothermal inputs (de Bar, Rampen, et al., 2019; Li et al., 2024; Schouten et al., 2008a; Umoh et al., 2022). The distribution of isoGMGTs (Figure 3) and isoGMGT biosynthesis genes in specific environments and archaea suggests that these lipids are restricted to anaerobic archaea (Garcia et al., 2024; Li et al., 2024).

Methylated isoGDGTs (Me-isoGDGTs) and methylated isoGMGTs (Me-isoGMGTs) contain one to three additional methyl groups in the biphytanyl or monoalkyl moieties, whose exact positions have not been determined except for the acyclic mono-methylated biphytane (Figure 2; Galliker et al., 1998; Knappy et al., 2015; Liu et al., 2012a; Lutnaes et al., 2007; Zhu et al., 2014b). Although these additional methyl groups have been proposed to represent an adaptation to low temperature (Knappy et al., 2015; Zhou & Dong, 2024), the occurrence of methylated isoGDGTs and isoGMGTs in hyperthermophilic archaea (Garcia et al., 2024; Liu et al., 2012a; Sollich et al., 2017) and their temperature-dependent distribution in hydrothermal sediments suggest that they might reflect an adaptation to high temperatures (Sollich et al., 2017). Methoxy isoGDGTs contain a methylation at the *sn*-1 hydroxyl group on one or two of the glycerol moieties (Figure 2; Elling et al., 2014; Zhu et al., 2014b). Although methoxy isoGDGTs can represent artifacts from acid hydrolysis using methanol (Ekiel & Sprott, 1992; Ferrante et al., 1988), they also occur in sediments and non-hydrolyzed *Nitrososphaeria* biomass (Figure 3); their roles in membrane homeostasis remain unknown (Elling et al., 2014; Zhu et al., 2014b).

Unsaturated isoGDGTs contain one to eight double bonds in the biphytanyl side chains and have been found only in anoxic marine sediments and water column as well as seep sediments (Zhu et al., 2014a, 2016), suggesting an anaerobic archaeal origin. Isoprenoid glycerol trialkyl glycerol tetraethers (isoGTGTs) have one biphytane and two phytane moieties, with isoGTGT-0 as the most common homolog (Figure 2; e.g., De Rosa et al., 1983; Hopmans et al., 2000). They have been detected in cultures (e.g., De Rosa et al., 1983; Elling et al., 2014; Schouten et al., 2008b; de la Torre et al., 2008) and marine sediments (Liu et al., 2012a); a role as an intermediate or side product in isoGDGT biosynthesis has been suggested (e.g., Lloyd et al., 2022).

Finally, isoprenoid butanetriol and pentanetriol dialkyl glycerol tetraethers (isoBDGTs and isoPDGTs) have one butanetriol and one pentanetriol moiety, respectively, replacing one of the isoGDGT glycerol moieties (Coffinet et al., 2020; Knappy et al., 2014; Zhu et al., 2014b). They have so far only been found in one pure culture, a methanogen (Figure 2; Becker et al., 2016; Coffinet et al., 2020) as well as an enrichment culture of *Bathymarchaeia* (Dong et al., 2025). Their distribution in the environment further supports *Bathymarchaeia* as a source of these lipids (Coffinet et al., 2020; Meador et al., 2015). Replacement of glycerol by butanetriol and pentanetriol also occurs in isoGTGTs and isoGMGTs, which have so far only been reported from a few marine sediments (de Bar, Rampen, et al., 2019; Knappy et al., 2014).

2.3. Diether Lipids

The first descriptions of archaeal diether lipids date back to the 1960s (De Rosa & Gambacorta, 1988; Kates et al., 1965; Sehgal et al., 1962). The most abundant and widespread diether lipid is archaeol (Figure 2), consisting of one glycerol moiety and two C₂₀ isoprenoidal (phytanyl) chains. It occurs in all or nearly all cultivated archaea, at least in trace amounts (Figure 3; Elling et al., 2017). Archaeol can include a methoxy group (Elling et al., 2014, 2015, 2017), one to two hydroxyl groups (Ferrante et al., 1988; Hinrichs et al., 2000; Rossel et al., 2008), and one to eight double bonds (e.g., Dawson et al., 2012; Hafenbradl et al., 1993; Zhu et al., 2016). Other common diether lipids include extended archaeol (De Rosa et al., 1982), which occurs prominently in alkaliphilic archaea but also some mesophilic and thermophilic archaea (e.g., Bale, Sorokin, et al., 2019; Becker et al., 2016; Dawson et al., 2012; Morii et al., 1999; Tindall et al., 1984; Yao et al., 2023). Extended hydroxylated archaeol is found in methanotrophic archaea (Stadnitskaia et al., 2008), macrocyclic archaeol with or without cyclopentane moieties is found in hyperthermophilic and methanotrophic archaea (Comita & Gagosian, 1983; Stadnitskaia et al., 2003), and acetylated archaeol in halophilic archaea (Kropp et al., 2022).

Isoprenoidal glycerol dibiphytanol diethers (isoGDDs) are ubiquitous in marine sediments (Hingley et al., 2024; Knappy & Keely, 2012; Liu et al., 2012b) and cultures of *Nitrososphaeria* and other GDGT-producing archaea (Bauersachs et al., 2015; Becker et al., 2016; Elling et al., 2015, 2017; Liu et al., 2012b; Meador et al., 2014). In comparison to isoGDGTs, they lack one glycerol moiety (Figure 2). IsoGDDs exhibit various structural modifications including the addition of one to two hydroxyl groups, an additional covalent bond between both di-alkanol moieties, and/or butanetriol and pentanetriol derivatives (Bauersachs & Schwark, 2016; Becker et al., 2016; de Bar, Rampen, et al., 2019; Liu et al., 2012a, 2016).

2.4. Intact Polar Lipids

Intact polar lipids (IPLs) occur in living cells and consist of a core lipid (either a diether or tetraether) attached to one or two polar headgroups (Figure 2; e.g., Sturt et al., 2004). These headgroups typically consist of either a phosphatidic, glycosidic, or combined glycosidic-phosphatidic moiety (e.g., Koga et al., 1993b, 1993a; Uda et al., 2001; Yoshinaga et al., 2011). Commonly observed phosphatidic headgroups include phosphatidylglycerol, phosphatidylethanolamine and phosphatidylserine (e.g., Koga & Morii, 2005; Sturt et al., 2004; Yoshinaga et al., 2011). Glycosidic headgroups typically comprise one to three glycosidically linked hexoses but can rarely also contain heptose moieties (Becker et al., 2016; Koga et al., 1993b; Koga & Morii, 2005). Combined glycosidic-phosphatidic headgroups typically are composed of a phosphate moiety bound to the lipid and one or more glycosidic moieties bound to the phosphate (e.g., Pitcher et al., 2011a; Shimada et al., 2002; Swain et al., 1997; Yoshinaga et al., 2011). Due to the large diversity of head groups among archaea, there are many combinations of head groups and core structures, and thus a large variety of IPLs is possible. In contrast, IPL assemblages in the marine water column are typically dominated by IPL-isoGDGTs and archaeols with monoglycosidic (1G), diglycosidic (2G) moieties, and sometimes triglycosidic (3G) headgroups (e.g., Lengger et al., 2012; Schubotz et al., 2009; Sturt et al., 2004). IsoGDGTs with phosphatidic and glycoposphatidic headgroups such as hexose-phosphohexose (HPH) are also abundant in seawater and marine sediments. Although IPL headgroup types can vary systematically on a taxonomic level in some archaeal clades (e.g., Koga et al., 1993b, 1993a; Koga & Morii, 2005), individual IPL headgroups can usually not be considered as associated with a specific clade. One exception is the use of HPH-crenarchaeol as a marker for living *Nitrososphaeria*, due to the specificity of the crenarchaeol core lipid (e.g., Lengger et al., 2012; Pitcher et al., 2011c). More diverse IPL assemblages are typically found in anoxic sediments and anaerobic zones such as in the Black Sea, which for example may contain abundant phosphatidic IPLs (e.g., Sollai et al., 2019b, 2019a; Yoshinaga et al., 2015; Zhu et al., 2024; Zhuang et al., 2016).

3. Biosynthesis of Archaeal Lipids

3.1. Biosynthesis of Diether and Tetraether Lipids

Pioneering early studies into the biosynthesis of archaeal membrane lipids focused on *sn*-2,3-di-*O*-phytanyl glycerol, that is, archaeol (Kates, 1993; Kates & Kushwaha, 1978). The biosynthesis of archaeol is now relatively well constrained (Jain, 2014; Koga & Morii, 2007; Villanueva et al., 2014; Figure 4). By contrast, significant progress has only recently been made in understanding the biosynthetic pathway of membrane-spanning isoGDGTs. The early hypothesis was that two archaeol diether lipids were combined to form a tetraether isoGDGT with 86 carbon atoms (Langworthy et al., 1982; Nemoto et al., 2003). This process involves the

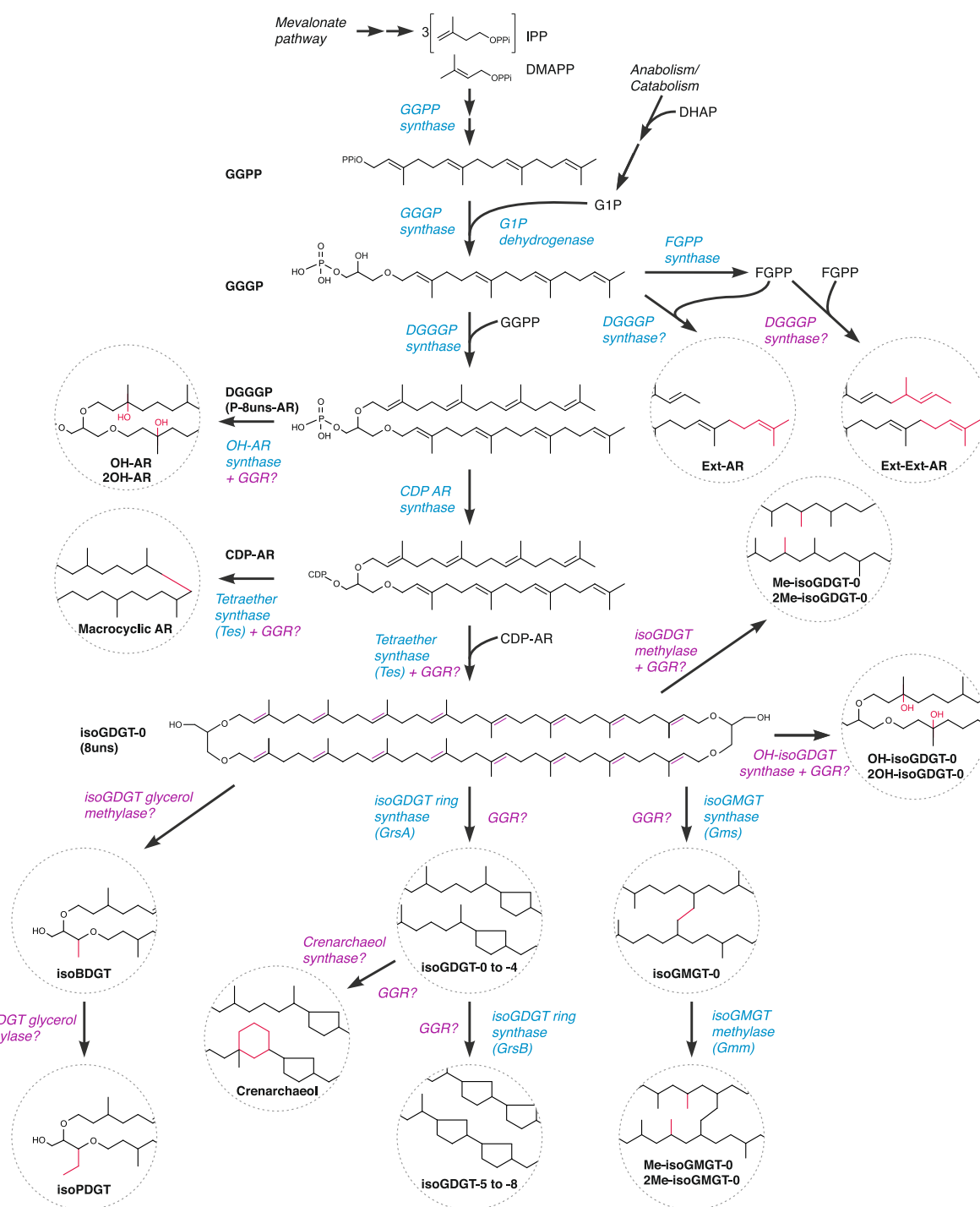


Figure 4.

formation of two sequential C–H activations on the terminal sp^3 carbons and requires challenging radical chemistry that was not known to occur in biological systems. The recent identification of Tetraether synthase (Tes), a radical SAM enzyme catalyzing the formation of membrane-spanning isoGDGTs through the combination of two archaeol molecules, has confirmed this mechanism (Figure 4; Lloyd et al., 2022; Zeng et al., 2022).

De Rosa, De Rosa, and Gambacorta (1977) originally proposed that the formation of cyclopentane moieties occurred via the internal cyclization of a methyl group with an sp^2 -hybridized carbon atom. This idea has recently been confirmed by the discovery of the two isoGDGT ring synthases (Zeng et al., 2019). One synthase (GrsA) leads to the formation of up to four cyclopentane moieties resulting in the formation of isoGDGT-1 to -4. The second enzyme (GrsB) acts after GrsA and catalyzes formation of cyclopentane units resulting in isoGDGT-5 to -8 (Figure 4).

Despite recent progress, many gaps exist in our understanding of isoGDGT biosynthetic pathways. For example, the order of biosynthetic steps such as saturation of double bonds by geranylgeranyl reductase (GGR) has not been established past the formation of archaeol (Figure 4). Although downstream enzymes such as Tes could potentially function with saturated precursors as suggested by Lloyd et al. (2022), experimental evidence suggests that Tes acts on terminal double bonds (Eguchi et al., 2003). Further, the biosynthetic pathway of various compounds such as OH-isoGDGTs, isoBDGTs and isoPDGTs remains unknown. Finally, the pathway for the formation of the cyclohexane moiety in isoGDGTs, leading to the formation of crenarchaeol (Sinninghe Damsté et al., 2002) and its isomer(s) (Liu et al., 2018; Sinninghe Damsté et al., 2018), remains unconstrained. However, as the stereochemistry of the four cyclopentane moieties in crenarchaeol is the same as in isoGDGT-4, the latter could be a biosynthetic precursor of crenarchaeol, through an additional internal cyclization reaction of one of the biphytanyl chains (Sinninghe Damsté et al., 2002) catalyzed by an, as yet, unknown enzyme.

3.2. Biosynthesis of Intact Polar Head Groups

Archaea produce a wide variety of polar headgroups (e.g., Koga et al., 1993b; Lipp & Hinrichs, 2009; Sturt et al., 2004) that have been suggested to modulate membrane properties (Gabriel & Chong, 2000). However, the biosynthetic pathways of intact polar lipids in archaea remain largely unconstrained. Only a few proteins have been characterized, with most studies characterizing enzymes catalyzing the biosynthesis of polar headgroups of archaeols (Jain et al., 2014; Morii et al., 2009; Morii & Koga, 2003). The biosynthesis of only one isoGDGT headgroup has been characterized so far, which is limited to the *Sulfolobales*, an order of thermoacidophilic archaea (Zeng et al., 2018). However, none of these specific headgroups occur in marine *Nitrososphaeria* (Elling et al., 2017; Pitcher et al., 2011a; Schouten et al., 2008b). Therefore, the biosynthetic pathways of polar headgroups found in these marine planktonic archaea remain to be identified.

4. Biological Sources of Tetraether Lipids in Ocean Waters

4.1. Archaeal Diversity in the Modern Ocean

There are four known major clades of planktonic archaea in today's oceans (Santoro et al., 2019). As reported taxonomic names of these marine archaeal groups frequently change due to updated phylogenies (Adam et al., 2017; Rinke et al., 2019; Spang et al., 2017), we use taxonomic names based on the genome taxonomy database (Parks et al., 2022) and summarize the original and new taxonomic classifications of archaeal groups related to marine planktonic archaea in Table 1. The major clades of marine planktonic archaea are generically

Figure 4. Biosynthesis pathway of archaeal diether (archaeols; ARs) and tetraether core lipids (isoGDGTs). Names of substrates and products are given in normal font; names of enzymes are in italics where blue color indicates known enzymes and purple color indicates unknown enzymes. Uncharacterized steps are marked with question marks. The sequence of biosynthetic steps from Tes onwards has not been constrained, in particular the saturation of double bonds by GGR and cyclization by GrsAB. Therefore, saturated instead of unsaturated precursors are possible. Note that lipid structural modifications may be combined, for example, methylated cyclized isoGMGTs or cyclized hydroxylated isoGDGTs. Abbreviations: IPP, isopentenyl-diphosphate; DMAPP, dimethylallyl pyrophosphate; DHAP, dihydroxyacetone phosphate; G1P, glycerol-1-phosphate; GGPP, geranylgeranyl diphosphate; GGGP, geranylgeranyl glycerol-1-phosphate; FGPP, farnesylgeranyl diphosphate; DGGGP, *sn*-2,3-di-*O*-geranylgeranyl glycerol-1-phosphate; CDP-AR, cytidine diphosphate archaeol; OH-AR, hydroxyarchaeol; Ext-AR, extended archaeol; Me-isoGDGT, methylated isoGDGT; isoBDGT, butanetriol dibiphytanyl glycerol tetraether; isoPDGT, pentanetriol dibiphytanyl glycerol tetraether; isoGMGT, glycerol monoalkyl glycerol tetraether (also called H-isoGDGT); Me-isoGMGT, methylated isoGMGT; OH-isoGDGT, hydroxylated isoGDGT; GGR, geranylgeranyl reductase. Individual biosynthetic steps are described in previous publications (Chen & Poulter, 1993; Garcia et al., 2024; Hemmi et al., 2004; Jain, 2014; Jain et al., 2014; Kakinuma et al., 1990; Li et al., 2024; Lloyd et al., 2022; Matsumi et al., 2011; Mori et al., 2015; Murakami et al., 2007; Tachibana et al., 1993, 2000; Villanueva et al., 2014; Zeng et al., 2019, 2022; Zhang & Poulter, 1993).

Table 1
Nomenclature of Original and New Taxonomic Groups of Archaea Discussed in Published Literature (Modified From Santoro et al., 2019)

General group name	ICNP validly published name ^a	Equivalent group name based on GTDB taxonomy ^b	Reclassified/reassigned group name based on current NCBI taxonomy ^c	Update reference(s)	Original group name	Original reference(s)
Marine Group I (MG-I)	Nitrososphaeria (class)	Thermoproteota (phylum); Nitrososphaeria (class); Nitrososphaerales (order); Nitrosopumilaceae (family)	Nitrososphaerota (Syn. Thaumarchaeota) (phylum) ^d Nitrosopumilales (order); Nitrosopumilaceae (family)	Brochier-Armanet et al. (2008), Oren & Garrity (2021) Könneke et al. (2005), Stieglmeier et al. (2014), Qin et al. (2017)	Crenarchaeota (phylum)	DeLong (1992), Fuhrmann et al. (1992)
Marine Group II (MG-II)	Methanobacteriota (phylum)	Thermoplasmata (phylum)	<i>Candidatus</i> Thermoplasmata (phylum)	–	Euryarchaeota (phylum)	DeLong (1992)
		Thermoplasmata (phylum); Poseidoniales (order); Poseidoniaceae (family)	<i>Candidatus</i> Thermoplasmata (phylum); <i>Candidatus</i> Poseidoniales (order); <i>Candidatus</i> Poseidoniaceae (family)	Rinke et al. (2019)	MG-IIa	Massana et al. (2000)
		Thermoplasmata (phylum); Poseidoniales (order); Thalassarchaeaceae (family)	<i>Candidatus</i> Thermoplasmata (phylum); <i>Candidatus</i> Poseidoniales (order); <i>Candidatus</i> Thalassarchaeaceae (family)	Martin-Cuadrado et al. (2015)	MG-IIb	Massana et al. (2000)
Marine Group III (MG-III)	Undefined	Undefined	<i>Candidatus</i> Thermoplasmata (phylum); <i>Candidatus</i> Thermoproteales (order)	Adam et al. (2017), Haro-Moreno et al. (2017)	MG-III	Fuhrman and Davis (1997)
		Halobacteriota (phylum); Halobacteria (class); Halobacteriales (order)	Epipelagoarchaeales and Bathypelagoarchaeales (proposed; orders/families)	–	MG-IV	López-García et al. (2001)
		Methanobacteriota (phylum); Methanobacteria (class)	Pontarchaea (proposed class)	–		
Methanogenic archaea (Methanogens)	Methanobacteriota (phylum)	Methanobacteriota (phylum); Methanobacteria (class)	Euryarchaeota (phylum); Methanobacteria* (class)		Euryarchaeota (phylum)	
		<i>Order-level lineages are the same as described in NCBI</i>	*Also known as Class I Methanogen			
		Halobacteriota (phylum); Halobacteria (class)	Order-level lineages: Methanobacteriales, Methanococcales, Methanopyrales			
		Halobacteriota (phylum); Halobacteria (class)	Euryarchaeota (phylum); Halobacteria** (class)		Euryarchaeota (phylum)	
		<i>Order-level lineages are the same as described in NCBI</i>	** Also known as Class II Methanogen			
		Halobacteriota (phylum); Syntropharchaeia (class); Alkanophagales (order)	Order-level lineages: Methanococcales, Methanopyrales			
Anaerobic methane oxidizing archaea (ANME-1)	Methanobacteriota (phylum)	Halobacteriota (phylum); Syntropharchaeia (class); Alkanophagales (order)	Euryarchaeota (phylum); Methanomicrobia (class); Methanophagales (order)	Adam et al. (2017)	Euryarchaeota (phylum)	

^aFollowing the International Code of Nomenclature of Prokaryotes (ICNP)'s list of validly published names as of 3 February 2024 (see Table 1; Oren, 2024). ^bLink to GTDB taxonomy database: <https://gtdb.ecogenomic.org/>; (Rinke et al., 2021). ^cLink to NCBI taxonomy database: <https://www.ncbi.nlm.nih.gov/Taxonomy/Browser/wwwtax.cgi>. ^dFormerly named Thaumarchaeota branching out from the NCBI phylum Crenarchaeota. The equivalent GTDB classification of the phylum Thaumarchaeota is now class Nitrososphaeria under the phylum Thermoproteota.

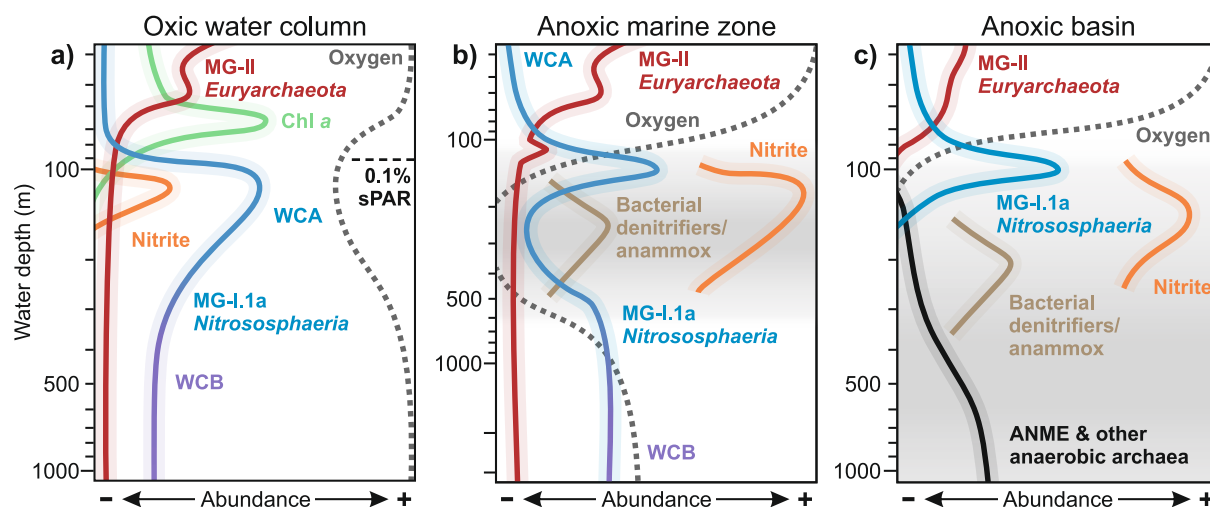


Figure 5. Conceptual water column profiles showing the distribution of Marine Group (MG) I.1a *Nitrososphaeria* and MG-II *Euryarchaeota* in the pelagic ocean. (a) Distribution for an idealized oxic water column, with MG-I.1a residing below the deep chlorophyll maximum at the base of the photic zone (0.1% surface photosynthetically active radiation, sPAR) near the primary nitrite maximum. MG-I.1a are further subdivided into water column cluster A (WCA) dominant in shallow waters and water column cluster B (WCB) dominant in deep water. Note that the relative and absolute depths of all features may vary strongly with oceanographic settings. (b, c) Distribution of MG-I.1a and MG-II as well as bacterial denitrifiers/anaerobic ammonium oxidizers (anammox) across an anoxic marine zone (oxygen minimum zone with anoxic core; e.g., eastern tropical Pacific; panel b) and an anoxic basin (e.g., Black Sea; panel c), where MG-I.1a predominantly occur in the suboxic transition zones. Figure based on Elling (2015) with data from (Belmar et al., 2011; Karner et al., 2001; Lam & Kuypers, 2011; Pitcher et al., 2011c; Podlaska et al., 2012; Schattenhofer et al., 2009; Sintes et al., 2016; Sollai et al., 2019a; Teira et al., 2006; Ulloa et al., 2012).

referred to as Marine Group I (MG-I), affiliated with the class *Nitrososphaeria*, and three lineages affiliated with the phylum *Euryarchaeota*: Marine Group II (MG-II, *syn. Candidatus Poseidoniales*), Marine Group III (MG-III), and Marine Group IV (MG-IV). MG-I is further subdivided into various subgroups, of which Group I.1a is dominant in the ocean, but also occurs in soils and freshwater. All cultivated MG-I are aerobic, chemoautotrophic nitrifiers (Santoro et al., 2019; Stahl & de la Torre, 2012), although some uncultivated lineages have been suggested to include heterotrophs (Aylward & Santoro, 2020). Specifically, MG-I oxidize ammonia into nitrite using O_2 as a source of energy, which is the first step in the biogeochemical process of nitrification, and use bicarbonate for carbon fixation (Könneke et al., 2005, 2014; Wuchter et al., 2003, 2006a). Studies on abundances of key archaeal genes in oxic marine water columns, for example, 16S rRNA and ammonia monooxygenase (*amoA*; encoding part of the enzyme mediating ammonia oxidation), revealed that MG-I.1a *Nitrososphaeria* (*Syn. Nitrosopumilales*) occupy the entire depth range in oxic water columns (Figure 5; e.g., Francis et al., 2005; Karner et al., 2001; Nunoura et al., 2015; Wuchter et al., 2006a). However, peak abundance of MG-I.1a is observed in the upper mesopelagic zone (i.e., near the base of the euphotic zone), where remineralization and ammonia release are highest (Santoro et al., 2019). MG-II *Poseidoniales* predominantly occupy the euphotic zone (for a review, see Santoro et al., 2019). In contrast to MG-I and MG-II archaea, the abundance and ecology of MG-III and MG-IV archaea is unclear. Genomic analyses of the physiology and metabolisms of MG-II, MG-III, and MG-IV suggest an aerobic, heterotrophic, and particle-attached lifestyle (Iverson et al., 2012; Martijn et al., 2020; Orsi et al., 2015).

MG-I.1a *Nitrososphaeria* are further subdivided into two depth-related phylogenetic clusters (Figure 5): “shallow” (Water Column Group A; WCA) and “deep” (Water Column Group B; WCB), based on *amoA* gene phylogenies (Francis et al., 2005; Sintes et al., 2013). The “shallow” clade (WCA) is generally present throughout the water column with the highest abundance in the epipelagic (0–200 m water depth) or upper mesopelagic (200–500 m water depth) waters (Figure 5a), and is thought to represent a high-ammonia concentration ecotype (Francis et al., 2005; Sintes et al., 2013). Species related to the genus *Nitrosopumilus* are sometimes included in the WCA cluster or separated into a third group related more closely to WCA than WCB. They are particularly abundant in environments with relatively high ammonia flux such as coastal regions (e.g., Hollibaugh et al., 2011, 2014) and brackish marginal seas (e.g., Labrenz et al., 2010; Wittenborn et al., 2023), but also hypersaline basins (Ngugi et al., 2015). The “deep” clade (WCB) dominates the meso- (200–1,000 m water depth) and bathypelagic (1,000–4,000 m water depth) zones and is thought to represent a more oligotrophic, low-ammonia concentration ecotype (Alves et al., 2018; Beman et al., 2012; Francis et al., 2005; Santoro et al., 2010; Sintes et al., 2013, 2016).

Although this depth zonation appears to be a consistent feature across ocean basins (Santoro et al., 2019), the depth of the transition between WCA versus WCB is spatially variable, likely due to large-scale features affecting water column structure, such as photic zone depth, upwelling zones, and subtropical gyres (e.g., Besseling et al., 2019; Santoro et al., 2017; Sintes et al., 2016).

Archaeal diversity and depth habitats in suboxic or anoxic water columns (Figure 5b) substantially diverge from those of oxic water columns (Figure 5a). In oxygen minimum zones (OMZs), MG-I.1a *Nitrososphaeria* are abundant across the oxic-anoxic transition but are absent within anoxic zones (Belmar et al., 2011; Bertagnolli & Stewart, 2018; Sollai et al., 2019b; Ulloa et al., 2012). Similarly, basins with euxinic conditions, such as the Black Sea, sub-basins within the Baltic Sea, and the Cariaco Basin, feature pronounced maxima in MG-I.1a *Nitrososphaeria* abundance and metabolic activity within the oxic-anoxic transition zone (e.g., Coolen et al., 2007; Labrenz et al., 2010; Pitcher et al., 2011c; Sollai et al., 2019a; Wakeham et al., 2004, 2007; Wittenborn et al., 2023). In these environments, MG-I.1a *Nitrososphaeria* are typically absent from the anoxic zone, whereas other archaea including methanogens and anaerobic methanotrophs can be abundant. The influence of anoxic marine zones (oxygen minimum zones with an anoxic core) and euxinic conditions upon the relative distribution of WCA versus WCB clades remains understudied (Lu et al., 2019).

4.2. Planktonic *Nitrososphaeria*—The Primary Source of Tetraether Lipids in the Modern Ocean

The diversity of marine archaea has resulted in a long-standing debate on the sources of isoGDGTs in the water column and consequently, marine sediments (e.g., Lincoln et al., 2014b, 2014a; Schouten et al., 2014; Turich et al., 2007). After early characterization of isoGDGTs from the sponge-symbiont *Cenarchaeum symbiosum* (DeLong et al., 1998; Sinninghe Damsté et al., 2002), studies of pure and enrichment cultures confirmed that (a) all MG-I.1a *Nitrososphaeria* of the *Nitrosopumilus* cluster and (b) the only available culture from the WCA cluster (*Ca. Nitrosopelagicus brevis*) biosynthesize isoGDGTs with zero to four cyclopentane moieties as well as crenarchaeol, its isomer and OH-isoGDGTs (DeLong et al., 1998; Elling et al., 2015, 2017; Pitcher et al., 2011a; Qin et al., 2015; Santoro et al., 2021; Schouten et al., 2008b; Sinninghe Damsté et al., 2002; Figure 3). Due to a lack of cultures, the lipid composition of WCB remains unknown.

Analysis of marine suspended particulate matter (SPM), particularly when coupled to marker gene abundances, revealed that isoGDGTs in marine environments are largely derived from MG-I.1a *Nitrososphaeria*. First, profiles of core- and IPL-isoGDGT abundance in SPM (and particularly IPL-crenarchaeol abundance, the most specific lipid biomarker for this group) show maxima below the photic zone (e.g., Basse et al., 2014; Coolen et al., 2007; Pitcher et al., 2011c; Wuchter et al., 2005), where ammonia oxidation rates are highest (Hurley et al., 2016). Second, isoGDGT abundances are correlated with MG-I.1a 16S rRNA gene abundance (Coolen et al., 2007; Pitcher et al., 2011c; Schouten et al., 2012; Sollai et al., 2019a, 2019b). Third, the major IPL-isoGDGTs in SPM are 1G-, 2G- and HPH-isoGDGTs, which are also the main IPLs in cultured MG-I.1a (Elling et al., 2017; Pitcher et al., 2011a; Schouten et al., 2008b).

While MG-I.1a *Nitrososphaeria* are clearly the dominant isoGDGT producers in oxic waters, the potential contributions of other planktonic archaeal groups have been debated. Unlike MG-I.1a, other planktonic archaeal groups such as MG-II, MG-III and MG-IV have not been cultured and, thus, their capacity to produce isoGDGTs in the marine water column is poorly constrained. Still, based on water column studies, MG-II Poseidoniales have been proposed as an additional source of isoGDGTs in the ocean water column (e.g., Lincoln et al., 2014b, 2014a; Turich et al., 2007; Wang et al., 2015). MG-II Poseidoniales are related to archaeal lineages with cultured representatives known to biosynthesize cyclopentane-containing isoGDGTs, such as the thermoacidophilic *Thermoplasmatales* (e.g., Uda et al., 2001) and the methanogenic *Methanomassiliicoccales* (e.g., Becker et al., 2016), suggesting that MG-II could be able to produce isoGDGTs. The observation that the IPL-derived isoGDGT concentration correlates with MG-II cell abundances in some areas, also suggested that MG-II are an additional source of isoGDGTs in marine waters (Li et al., 2021; Lincoln et al., 2014a, 2014b; Ma et al., 2020; Turich et al., 2007). However, this interpretation has been challenged (e.g., Schouten et al., 2014), and other studies of IPL-isoGDGTs from marine waters dominated by MG-II suggests that MG-II do not contribute to the sedimentary record of isoGDGTs (Besseling et al., 2020; Villanueva et al., 2017). Absence of isoGDGT production in MG-II is further supported by recent insights based on isoGDGT biosynthetic genes. First, the *Tes* homolog is absent in metagenome-assembled genomes (MAGs) of MG-II (except for a single MG-II MAG), suggesting that they mostly do not produce isoGDGTs (Zeng et al., 2022). Second, *grsA*, the gene responsible for the biosynthesis

of isoGDGTs with 0–4 cyclopentane moieties (see Figure 4), is present in MG-I but absent from MG-II and MG-III MAGs, suggesting that neither produces isoGDGTs with cyclopentane moieties (Zeng et al., 2019). Although the presence of isoGDGT biosynthetic genes in MG-IV has not been studied, this group is very rare throughout the ocean (e.g., Besseling et al., 2019; López-García et al., 2001). Collectively, these observations indicate that MG-II, MG-III, and MG-IV are unlikely to be (significant) sources of cyclized isoGDGTs in the ocean.

Although MG-I.1a are the dominant producers of isoGDGTs in the oxic marine water column, WCA and WCB clusters may differ in the relative proportions of individual isoGDGTs in their membranes (e.g., Besseling et al., 2019; Hernández-Sánchez et al., 2014). For example, a globally observed increase in the isoGDGT-2/isoGDGT-3 ratio in SPM below a water depth of ~200 m is commonly attributed to a higher proportion of isoGDGT-2 produced by WCB (e.g., Besseling et al., 2019; Hernández-Sánchez et al., 2014; Kim et al., 2016; Rattanasriampaipong et al., 2022). Although most studies on isoGDGT-2/isoGDGT-3 ratios did not provide genetic data to support a causal link between isoGDGT-2/isoGDGT-3 ratios and WCB abundance, Besseling et al. (2019) showed that an increase in the isoGDGT-2/isoGDGT-3 ratio in the Mediterranean Sea coincides with higher relative abundance of WCB. Villanueva et al. (2015) suggested that distinct sequence motifs found in the biosynthesis protein DGGP synthase (producing the isoGDGT precursor archaeol) found below 500 m water depth could also explain the observed elevated isoGDGT-2/isoGDGT-3 ratios due to a genetic control of lipid composition. Yet, it remains unclear why isoGDGT-2/isoGDGT-3 ratios in water depths below ~200 m vary strongly in magnitude across different ocean basins (summarized by Besseling et al., 2019).

In anoxic or euxinic settings, isoGDGTs may be produced by additional groups of archaea. The best-studied example is the modern Black Sea (Figure 5c), where anaerobic archaea including methanotrophs produce isoGDGTs with up to 4 cyclopentane moieties in the anoxic part of the water column (e.g., Schubert et al., 2006; Schubotz et al., 2009; Sollai et al., 2019a; Wakeham et al., 2003, 2004), in addition to other diether and tetraether lipids (e.g., Sollai et al., 2019a; Zhu et al., 2016, 2024). This is also found in other euxinic basins and open-ocean oxygen minimum zones (e.g., Sollai et al., 2019b; Wakeham et al., 2004, 2012; Xie et al., 2014; Zhu et al., 2016). For the Black Sea and Cariaco Basin, compound-specific $\delta^{13}\text{C}$ analysis of isoGDGT-derived biphytanes indicate that the overall contribution of these anaerobic isoGDGT producers to the sedimentary signal is limited, possibly due to inefficient export to sediments (Wakeham et al., 2003, 2004; see Section 6).

In summary, while anoxic and euxinic environments may have additional archaeal sources of isoGDGTs, the analysis of core- and IPL-isoGDGTs from cultures and SPM indicates that the sedimentary isoGDGT record in most marine settings, and thus TEX_{86} , is primarily contributed by planktonic MG-I.1a *Nitrososphaeria* in the overlying oxic water column (discussed in detail in Sections 6–8).

5. IsoGDGT-Based Marine Temperature Proxies

5.1. IsoGDGTs as Marine Temperature Proxies

Schouten et al. (2002) first demonstrated that the weighted average number of cyclopentane moieties found in isoGDGTs in marine surface sediments had a strong relationship ($r = 0.8$) with annual mean SST (derived from the nearest one-degree grid in the 1998 World Ocean Atlas; WOA98; Levitus et al., 1998). This relationship was substantially improved (i.e., to $r = 0.96$) by using the TEX_{86} ratio (Equation 2), which includes the crenarchaeol isomer but is not a direct reflection of the number of cyclopentane moieties found in isoGDGTs. Using a global surface sediment database ($n = 44$), TEX_{86} was calibrated to SST and subsurface (i.e., at 100 m) temperature using a linear regression model (Schouten et al., 2002). Kim et al. (2008) expanded the original surface sediment data set ($n = 223$) and identified a non-linear relationship between TEX_{86} and SST in polar regions. To resolve this, the TEX_{86} -SST relationship was recalibrated using a linear regression model without sites where SST was $<5^\circ\text{C}$ (Kim et al., 2008). This calibration also excluded samples from the Red Sea, a narrow, semi-enclosed basin characterized by high temperatures and salinity that contains a unique endemic archaeal population (Ionescu et al., 2009; Qian et al., 2011). In the Red Sea, TEX_{86} values are anomalously high (Kim et al., 2008; Trommer et al., 2009) and surface sediments contain a higher relative abundance of crenarchaeol isomer compared to other sites from similar latitudes.

A number of non-linear calibrations were subsequently proposed (e.g., Kim et al., 2010; Liu et al., 2009). The most widely used non-linear calibration, $\text{TEX}_{86}^{\text{H}}$ (Kim et al., 2010), uses a revised formulation of TEX_{86} :

$$\text{TEX}_{86}^{\text{H}} = \log_{10} \frac{[\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol isomer}]}{[\text{isoGDGT} - 1] + [\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol isomer}]} \quad (3)$$

The $\text{TEX}_{86}^{\text{H}}$ calibration assumes an exponential relationship with SST (i.e., TEX_{86} becomes less sensitive at higher SSTs) and employs a common logarithmic ($\log_{10}$) transformation (Kim et al., 2010). This calibration, with a residual error of 2.5°C, excludes surface sediments from the Red Sea and those from areas where SST < 5°C. In the modern surface sediment calibration range (~5–30°C) linear (e.g., Kim et al., 2008; Schouten et al., 2002) and non-linear calibrations (e.g., Kim et al., 2010) reconstruct similar temperatures, but they increasingly diverge when they approach the upper limit of the modern calibration range (i.e., instrumental SST > 30°C). Several indicators for a non-linear relationship between temperature and isoGDGT distributions exist in the core-top surface sediment data set (e.g., Cramwinckel et al., 2018; Dunkley Jones et al., 2020; Fokkema, Agterhuis, et al., 2024; Kim et al., 2010). As such, a non-linear exponential relationship has often been used for temperature reconstructions during the Neogene (23–2.6 Ma), Paleogene (66–23 Ma) and Cretaceous (145–66 Ma; e.g., Linnert et al., 2014; Littler et al., 2011; Liu et al., 2009; van der Weijst et al., 2022). Several studies have shown that the temperatures derived from non-linear calibrations often agree more closely with SST estimates from independent inorganic proxies, which may support a non-linear relationship between temperature and TEX_{86} (e.g., de Bar, de Nooijer, et al., 2019; Cramwinckel et al., 2018; Frieling et al., 2017; Liu et al., 2009; Woelders et al., 2018). However, those studies also show that non-linear calibrations yield lower (sub)tropical SSTs than linear models, further flattening equator-to-pole SST gradients during past warm climates. As marine sediments of Paleogene and Cretaceous age are often characterized by very high TEX_{86} values, they require extrapolation far beyond the modern surface sediment calibration data set and require careful consideration of the most appropriate calibration model(s).

Kim et al. (2010) also introduced another index, $\text{TEX}_{86}^{\text{L}}$, which excludes isoGDGT-3 from the numerator and excludes the crenarchaeol isomer entirely. $\text{TEX}_{86}^{\text{L}}$ assumes an exponential relationship with SST, but unlike $\text{TEX}_{86}^{\text{H}}$, was based on the entire surface sediment data set (except the Red Sea) available at that time. $\text{TEX}_{86}^{\text{L}}$ was initially suggested for application in colder climates (i.e., where SST < 15°C). This approach has been applied in high-latitude environments (e.g., Harning et al., 2019; Meyer et al., 2016; Sangiorgi et al., 2018; Vorrath et al., 2023) and sites where the relative abundance of the crenarchaeol isomer is low and the water column is shallow (i.e., the Baltic Sea; Kabel et al., 2012; Wittenborn et al., 2022). Low relative abundance of the crenarchaeol isomer in the Baltic Sea is likely related to its endemic population of *Nitrososphaeria* (Berg, Listmann, et al., 2015; Berg, Vandieken, et al., 2015; Labrenz et al., 2010; Wittenborn et al., 2023). However, as $\text{TEX}_{86}^{\text{L}}$ excludes isoGDGT-3 from the numerator, it is more sensitive to changes in isoGDGT-2/isoGDGT-3 ratios (Taylor et al., 2013). Application of $\text{TEX}_{86}^{\text{L}}$ is therefore not recommended outside the Baltic Sea and caution is needed when applying this proxy to polar regions (Bijl et al., 2025; Fietz et al., 2020).

Tierney and Tingley (2014) noted that the (non-linear) Kim et al. (2008, 2010) calibration models exhibited large residuals, resulting in overestimation of temperatures at high latitudes and underestimation at low latitudes. This is because these calibrations were affected by regression dilution bias (Tierney & Tingley, 2014) owing to the treatment of TEX_{86} as an independent variable rather than a dependent variable. Large residuals >> 1σ are observed for some locations in a greatly expanded data set ($n > 2000$; Figure 6). For example, sediments from many tropical localities have residuals that are as high as found in surface sediments from the Red Sea, suggesting that excluding the Red Sea from global calibrations may be somewhat arbitrary. It is evident from the latitudinal distribution of TEX_{86} values and residuals that regressions with strongly diverging slopes could be constructed for different latitudinal bands or regions (Figures 6b and 6c). Building on such observations, Tierney and Tingley (2014) proposed a spatially-varying Bayesian regression model (BAYSPAR). This approach assumes a linear relationship between TEX_{86} and SST but takes into account all data from the surface sediment data set except data > 70°N (including the Red Sea; Tierney & Tingley, 2014) and varies the regression slope and intercept across space to account for regional differences in ecological and environmental factors. To quantify past temperatures, BAYSPAR searches the modern surface sediment data set for TEX_{86} values that are similar to the measured TEX_{86} value within a user-specified tolerance and draws regression parameters from these modern “analogue” locations. This approach also yields uncertainty bounds that reflect spatial differences in the slope and intercept terms and the error variance of the regression model and can be used to estimate uncertainty beyond the modern calibration range. BAYSPAR assumes a linear correlation beyond the modern-calibration data set (> 30°C) and as such can result in very high (> 40°C) SST estimates during past greenhouse climates (O’Brien et al., 2017). For a given TEX_{86} value, BAYSPAR will often yield higher SSTs than $\text{TEX}_{86}^{\text{H}}$ but lower SSTs than other linear TEX_{86}

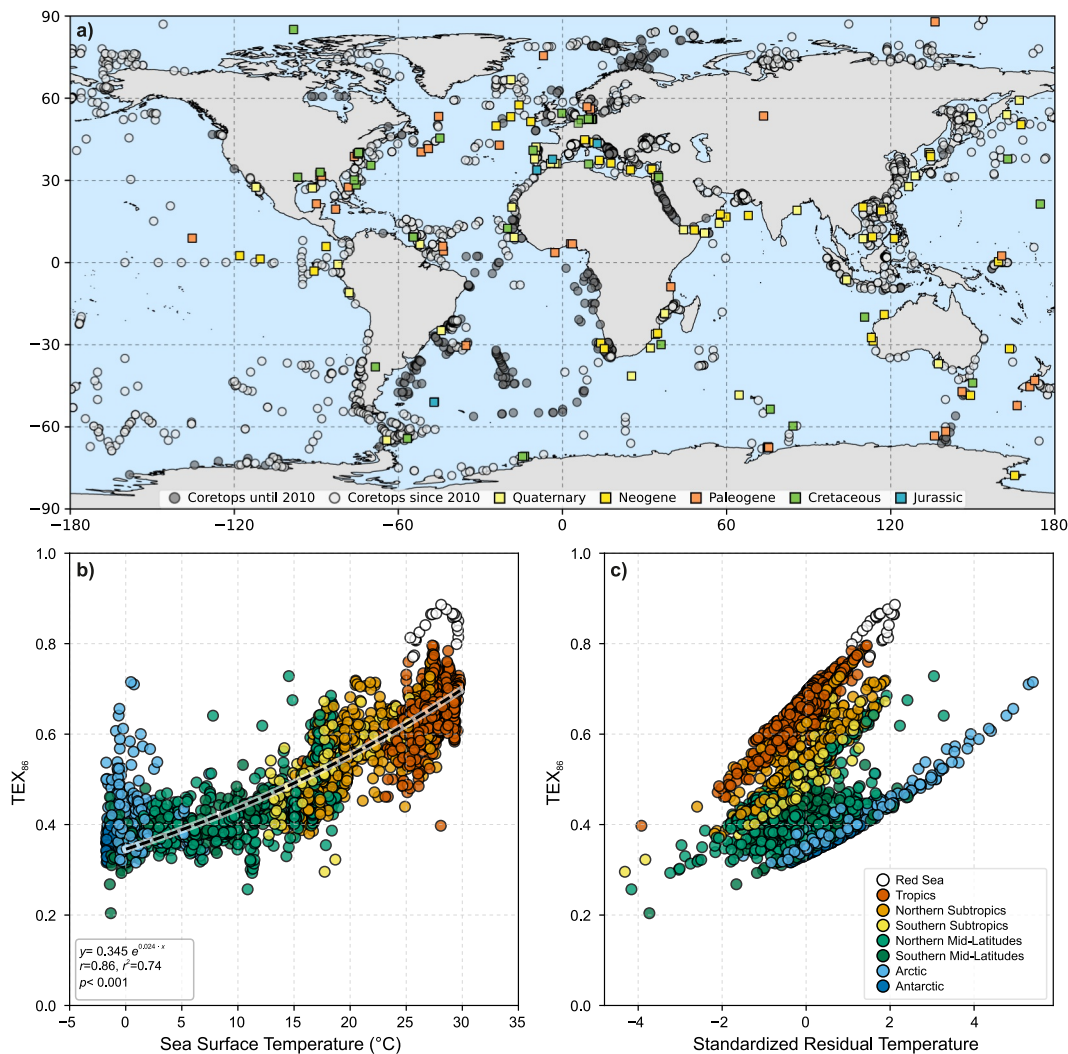


Figure 6. (a) Location of surface sediments used for TEX₈₆ calibrations ($n = 2082$; compiled by Rattanasriampaipong et al., 2025) and core sites used for TEX₈₆ SST reconstructions compiled in the PhanSST database (Judd et al., 2022). Surface sediments represent individual modern sediments whereas the PhanSST entries represent core locations from which time-resolved downcore records have been generated for paleo-SST reconstructions. (b) Correlation of TEX₈₆ in surface sediments with SST using an exponential regression (SST obtained from the nearest World Ocean Atlas 2023 SST data point for each location; Locarnini et al., 2024). Data are colored by latitudinal bands (Arctic: $\geq 66.5^\circ\text{N}$; Antarctic: $\geq 66.5^\circ\text{S}$; Southern Mid-Latitudes: $44\text{--}66.5^\circ\text{S}$; Northern Mid-Latitudes: $40\text{--}66.5^\circ\text{N}$; Southern Subtropics: $23.5\text{--}40^\circ\text{S}$; Northern Subtropics: $23.5\text{--}40^\circ\text{N}$; Tropics: $23.5^\circ\text{S}\text{--}23.5^\circ\text{N}$; Red Sea plotted separately). (c) Standardized residual temperatures ($[\text{SST}_{\text{TEX86}} - \text{SST}_{\text{actual}}] / \text{standard deviation of residuals}$) based on the global logarithmic regression from panel (b). Surface sediment data are divided into those published up to 2010 and therefore included in the original TEX₈₆^H and TEX₈₆^L calibrations (Kim et al., 2008, 2010; Schouten et al., 2002) and those published since 2010 (Ceccopieri et al., 2018; Chen et al., 2018; Hagemann et al., 2023; Harning et al., 2019, 2023; Jaeschke et al., 2017; Kaiser et al., 2015; Kim et al., 2015; Kusch et al., 2016; Lamping et al., 2021; Lo et al., 2018; Pan et al., 2016; Rattanasriampaipong et al., 2025; Richey & Tierney, 2016; Rodrigo-Gámiz et al., 2015; Schukies, 2018; Sinninghe Damsté et al., 2022; Tierney et al., 2015; Tierney & Tingley, 2014, 2015; Varma et al., 2024b; Wei et al., 2020; Yang et al., 2018). The data set was not filtered but quality metrics (BIT, MI, %isoGDGT-0, ΔRI) are provided in Figure 14 and in the original data set of Rattanasriampaipong et al. (2025).

calibrations applied in greenhouse climates (i.e., TEX₈₆-linear; see Inglis & Tierney, 2020 for further discussion; O'Brien et al., 2017).

A recent machine learning approach (OPTiMAL) takes into account all six major isoGDGTs (including isoGDGT-0 and crenarchaeol; Dunkley Jones et al., 2020). Using a Gaussian processes (GP) emulator to optimize temperature estimation from previous surface sediment calibration data sets (e.g., Kim et al., 2010; Tierney & Tingley, 2015 and references therein) this approach avoids the dimensionality reduction of standard indices and ratios (Dunkley Jones et al., 2020). The approach requires no a priori assumption about the form of the isoGDGT-SST relationship, which is optimized with a set of learned functions across the modern calibration. OPTiMAL can

evaluate how a fossil isoGDGT assemblage compares to the modern calibration set by using its learned Gaussian-process (GP) functions to compute a temperature-sensitivity weighted distance in isoGDGT space. The distance of closest approach between a fossil isoGDGT assemblage and any modern isoGDGT assemblage is termed D_{nearest} . Assemblages with $D_{\text{nearest}} > 0.5$ are considered outside the calibration envelope and are not used for SST estimation by OPTiMAL. OPTiMAL has been applied to estimate SST during the late Pleistocene to Holocene (last 11,700 years) and Paleocene-Eocene Thermal Maximum (~56 Ma; Dunkley Jones et al., 2020). However, the OPTiMAL approach is fundamentally constrained within the parameter space of the modern calibration and has very little-to-no predictive power outside of the modern calibration data (i.e., $>30^{\circ}\text{C}$).

With the exception of upwelling zones and polar regions, SST and subsurface temperatures are closely related in the modern ocean, implying that TEX_{86} could also be calibrated to subsurface temperatures (Schouten et al., 2002). $\text{TEX}_{86}^{\text{H}}$ and $\text{TEX}_{86}^{\text{L}}$ have both been calibrated to shallow subsurface temperature and assume constant production within the top 200 m of the water column (Kim et al., 2008, 2010, 2012a). TEX_{86} has also been calibrated to shallow subsurface temperatures (0–200 m) using a Bayesian approach (BAYSPARsubT; Tierney & Tingley, 2015). This calibration uses the original TEX_{86} index but assumes maximum isoGDGT export occurs at ~50 m water depth. Ho and Laepple (2016) recalibrated TEX_{86} to subsurface temperature but unlike the calibration models described above (Kim et al., 2008, 2010; Tierney & Tingley, 2015), this calibration (HL16) represents an ensemble of regressions that include isoGDGT export at deeper water depths (up to 950 m; Ho & Laepple, 2016). However, both Tierney et al. (2017) and Ho and Laepple (2016, 2017) emphasized that any chosen subsurface calibration needs to be adequate for the water depth of the paleorecord it is applied to, as applying a deep water calibration to shallow water paleorecords may lead to erroneous results. Moreover, as isoGDGT concentration typically peaks at and/or below the nitracline (~50–250 m depth) and that the majority of isoGDGT export likely occurs in the surface ocean (see Section 6.2), substantial deep export (i.e., up to 950 m or deeper) is unlikely.

The aforementioned subsurface temperature calibrations are thus based on temperatures from a fixed depth range (e.g., 0–200 m) and do not account for spatial variability in the depth of the surface mixed layer and thermocline, which are important variables determining the niche of *Nitrososphaeria* in the marine water column. Changes in the niche of *Nitrososphaeria* can bias temperature estimates—yielding artificially low values in upwelling regions where the thermocline is shallower, and overly high values in subtropical gyres where the thermocline extends well below 200 m (Rattanasriampaipong et al., 2025). To ascertain whether a surface or subsurface calibration is more appropriate, we require an improved mechanistic understanding of isoGDGT export production (see Section 6). Although TEX_{86} in globally distributed marine surface sediments is correlated with sea surface temperature as well as subsurface temperatures, large residuals with uncertain origins remain (Figure 6c). These residuals are potentially due to spatially varying patterns in community composition, physiological factors, exogenous sources, and water-depth dependent production and export, that are explored further below (see Sections 6–9).

5.2. Hydroxylated isoGDGTs as Marine Temperature Proxies

A major uncertainty in the global surface sediment TEX_{86} calibration is the weak relationship between TEX_{86} and SST at lower (typically $<10^{\circ}\text{C}$) temperatures (e.g., Ho et al., 2014; Kim et al., 2008, 2010; Tierney & Tingley, 2015), limiting the application of TEX_{86} in polar regions (Fietz et al., 2020). While $\text{TEX}_{86}^{\text{L}}$ (Kim et al., 2010) was originally used to reconstruct SST in colder polar regions, this index is no longer recommended except in specific environments (e.g., the Baltic Sea; see Section 5.1).

More recently, alternative temperature metrics have been developed using hydroxylated isoGDGTs (OH-isoGDGTs). OH-isoGDGTs are particularly abundant (relative to all isoGDGTs) in polar sediments (Fietz et al., 2013, 2020; Harning et al., 2023; Harning & Sepúlveda, 2024; Huguet et al., 2013; Varma et al., 2024b) and may represent a mechanism for membrane adaptation at low temperatures (Fietz et al., 2013, 2020; Huguet et al., 2013). OH-isoGDGTs are so far known to be biosynthesized by a small subset of archaea, including all mesophilic group I.1a *Nitrososphaeria* (Bale, Palatinszky, et al., 2019; Elling et al., 2017; Varma et al., 2024a), but also a thermophilic methanogen (Liu et al., 2012c) and a freshwater methanotroph (Figure 3; Kurth et al., 2019).

The abundance of OH-isoGDGTs relative to non-hydroxylated isoGDGTs in marine surface sediments increases at lower temperatures (Figure 7a; Fietz et al., 2013, 2020; Harning & Sepúlveda, 2024; Harning et al., 2023; Huguet et al., 2013; Lü et al., 2015) and there is a negative correlation between OH-isoGDGT-0 and SST (Fietz et al., 2016; Varma et al., 2024b). This led to a revised formulation of TEX_{86} that includes OH-isoGDGT-0 in the denominator (Figure 7b; Varma et al., 2024b):

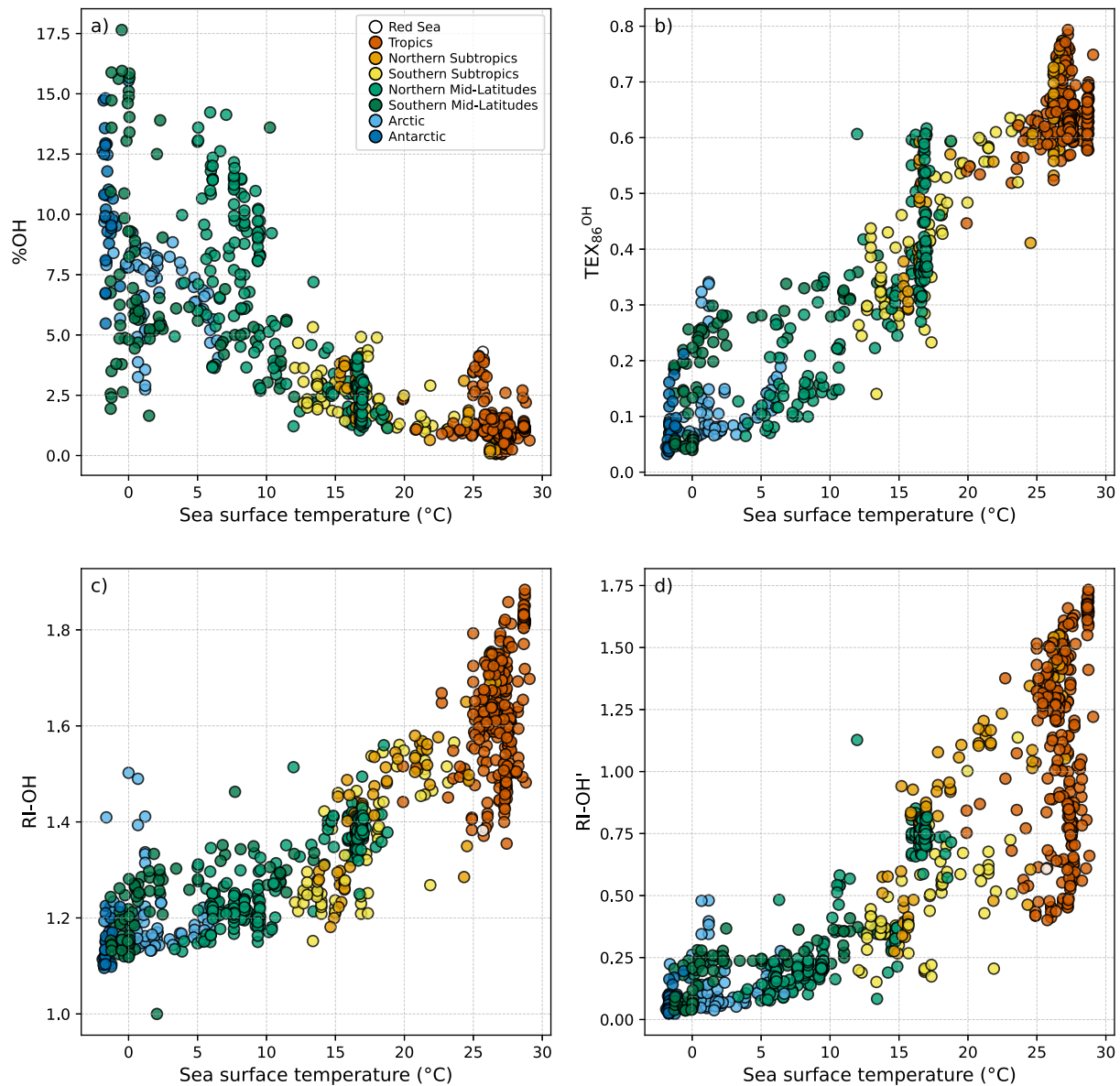


Figure 7. OH-isoGDGTs in global surface sediments plotted against annual mean sea surface temperature ($n = 872$). (a) relative abundance of OH-isoGDGTs (%OH), (b) $\text{TEX}_{86}^{\text{OH}}$ (c) ring index of OH-isoGDGTs (RI-OH), (d) modified RI-OH (RI-OH'). OH-isoGDGT data from (Fietz et al., 2013, 2016; Huguet et al., 2013; Kaiser & Arz, 2016; Lamping et al., 2021; Lü et al., 2015; Varma et al., 2024b; Wei et al., 2020; Yang et al., 2018). Sea surface temperature data from (Locarnini et al., 2019). Data are colored by latitudinal bands (Arctic: $\geq 66.5^\circ\text{N}$; Antarctic: $\geq 66.5^\circ\text{S}$; Southern Mid-Latitudes: $44\text{--}66.5^\circ\text{S}$; Northern Mid-Latitudes: $40\text{--}66.5^\circ\text{N}$; Southern Subtropics: $23.5\text{--}40^\circ\text{S}$; Northern Subtropics: $23.5\text{--}40^\circ\text{N}$; Tropics: $23.5^\circ\text{S}\text{--}23.5^\circ\text{N}$; Red Sea plotted separately).

$$\text{TEX}_{86}^{\text{OH}} = \frac{[\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol isomer}]}{[\text{isoGDGT} - 1] + [\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol isomer}] + [\text{OH} - \text{isoGDGT} - 0]} \quad (4)$$

This new index improves the temperature sensitivity in regions with mean annual SST between 5 and 15°C and in polar regions (Varma et al., 2024b). The mechanism that underpins the empirical correlation between $\text{TEX}_{86}^{\text{OH}}$ index and SST is uncertain. However, molecular dynamics simulations suggest that the additional hydroxyl group(s) form hydrogen bonds with adjacent lipid sugar headgroups and water, enlarging the polar headgroup

area. Hydroxylation also perturbs chain packing, with disorder propagating along the alkyl chains, increasing membrane fluidity (Huguet et al., 2017).

In marine surface sediments, the weighted average number of cyclopentane moieties of OH-isoGDGTs also varies as a function of temperature (expressed via the ring index of hydroxylated tetraethers; RI-OH and RI-OH'; Figures 7c and 7d; Fietz et al., 2013; Lü et al., 2015; Varma et al., 2024b):

$$RI - OH = \frac{[OH - isoGDGT - 1] + 2 \times [OH - isoGDGT - 2]}{[OH - isoGDGT - 1] + [OH - isoGDGT - 2]} \quad (5)$$

$$RI - OH' = \frac{[OH - isoGDGT - 1] + 2 \times [OH - isoGDGT - 2]}{[OH - isoGDGT - 0] + [OH - isoGDGT - 1] + [OH - isoGDGT - 2]} \quad (6)$$

RI-OH is suggested for use when SSTs >15°C, while RI-OH' is more suitable in colder and polar environments where SST <15°C (Lü et al., 2015). Both RI-OH and RI-OH' have been increasingly applied to diverse marine environments, especially over Quaternary timescales (i.e., 2.58 Ma to present; e.g., Davtian et al., 2019, 2021; Kremer et al., 2018; Morcillo-Montalbá et al., 2021; Santos et al., 2026; Suzuki et al., 2025; Vorrath et al., 2023), where their records often show good correspondence with other paleotemperature proxies. OH-isoGDGTs are thought to be relatively labile and may be more susceptible to degradation compared to isoGDGTs. However, the oldest known occurrence of OH-isoGDGTs is currently ~94 Ma (Connock et al., 2022), implying that OH-isoGDGT-based proxies warrant further attention in Mesozoic and early Cenozoic environments.

Unlike TEX₈₆ (see Sections 7 and 8), relatively little is known about non-thermal effects on OH-isoGDGT proxies. Culture experiments support a relationship between temperature and the relative abundance of OH-isoGDGTs as well as their relative number of cyclopentane moieties (Varma et al., 2024a). However, strong differences in the OH-isoGDGT content between closely related strains suggest additional factors exert a control besides temperature (Elling et al., 2015, 2017; Varma et al., 2024a). Furthermore, correlations of OH-isoGDGT cyclization with temperature in cultures are strongly offset from global marine surface sediment calibrations (Varma et al., 2024a). Environmental factors such as nitrate concentrations (as a possible indicator of nutrient levels), dissolved oxygen levels, and water-column stratification have been identified as controls on OH-isoGDGT distributions in the subpolar North Atlantic (Harning & Sepúlveda, 2024). Similarly, salinity has been suggested to strongly influence OH-isoGDGT cyclization in Baltic Sea surface sediments and paleorecords, potentially due to an effect of salinity on MG-I.1a community composition (Sinninghe Damsté et al., 2022). Like TEX₈₆, OH-isoGDGT-based proxies may be affected by water depth, although data to support this is currently limited (Fietz et al., 2016; Varma et al., 2024b, 2024c; Xiao et al., 2023b). Such an effect of water depth was observed for TEX₈₆^{OH} in sediments from the Mediterranean Sea and Red Sea, suggesting an influence of community composition on TEX₈₆^{OH} (Varma et al., 2024c). However, RI-OH and RI-OH' ratios were not affected by water depth in either Red Sea or Mediterranean sediments (Varma et al., 2024b, 2024c). Terrigenous input (Varma et al., 2025) and/or input of additional archaeal groups besides *Nitrososphaeria* such as methanogens and/or methanotrophs (Guan et al., 2024) may contribute to the sedimentary OH-isoGDGT pool, but their contributions and impacts on OH-isoGDGT proxies are currently unconstrained.

In summary, OH-isoGDGTs are a promising approach that can be employed alongside TEX₈₆ to reconstruct surface ocean temperatures, especially in the low temperature range (<10°C) where TEX₈₆ has traditionally struggled. However, the impact of non-thermal factors and community composition on OH-isoGDGT-derived temperature estimates requires further work.

6. isoGDGT Production and Export Depth

6.1. Evaluating isoGDGT Production and Export Using SPM and Sediment Traps

Constraining the depth of archaeal lipid export production in the water column is essential for applying isoGDGT-based paleoclimate proxies (e.g., TEX₈₆) in marine sediments and exploring whether sea surface temperature or subsurface temperature calibrations are more appropriate (see Section 5). Suspended Particulate Matter (SPM) profiles of IPL and core lipids suggest that isoGDGT production occurs throughout the marine water column, but isoGDGT concentrations typically peak near the base of the photic zone, at and/or below the nitracline (~50–250 m depth; Figures 8 and 9; Basse et al., 2014; Besseling et al., 2019; Coolen et al., 2007; Guo

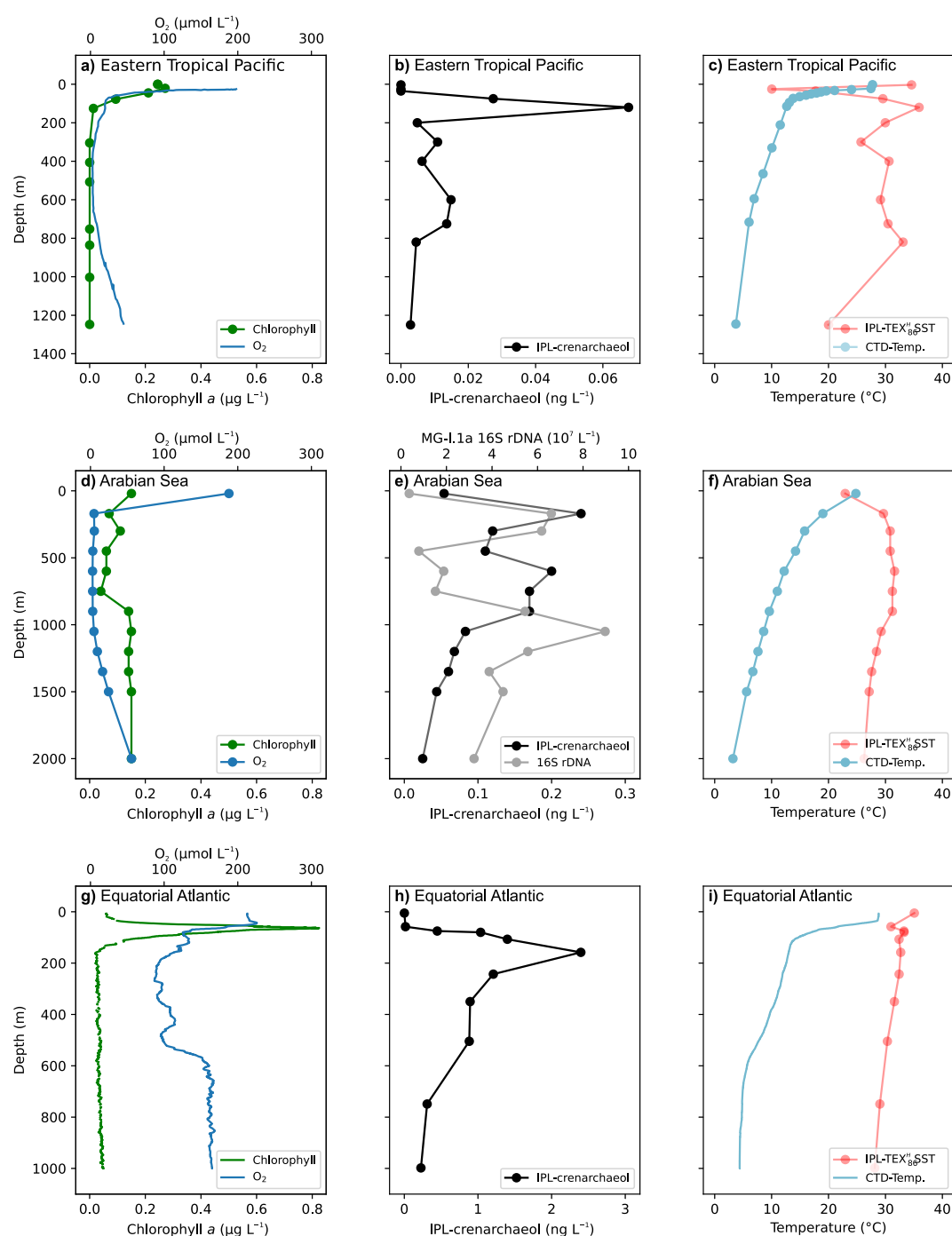


Figure 8. Examples of the co-variation of IPL-crenarchaeol concentrations (summed monoglycosyl-, diglycosyl-, and hexose-phosphohexose-crenarchaeol), MG-I.1a abundance (16S rDNA copies; only Arabian Sea) and TEX₈₆^H-derived SST in suspended particulate matter with oceanographic parameters in the Eastern Tropical North Pacific (a–c; Xie et al., 2014; Zhu et al., 2016), the Arabian Sea oxygen minimum zone (d–f; Pitcher et al., 2011c; Schouten et al., 2012), and the equatorial Atlantic Ocean upwelling zone (g–i; Hurley et al., 2018). Note that these data were generated using different extraction and analytical methods and that crenarchaeol concentrations may therefore not be comparable between sites.

et al., 2024; Hernández-Sánchez et al., 2014; Hurley et al., 2018; Ingalls et al., 2012; Jia et al., 2017; Schouten et al., 2012; Spencer-Jones et al., 2021; Wittenborn et al., 2023; Wuchter et al., 2005; Xie et al., 2014). At most locations studied so far, SPM-based TEX₈₆ values are correlated with in situ temperatures only in the uppermost water column (i.e., within the photic zone) where MG-I.1a and isoGDGTs are of relatively low abundance. In

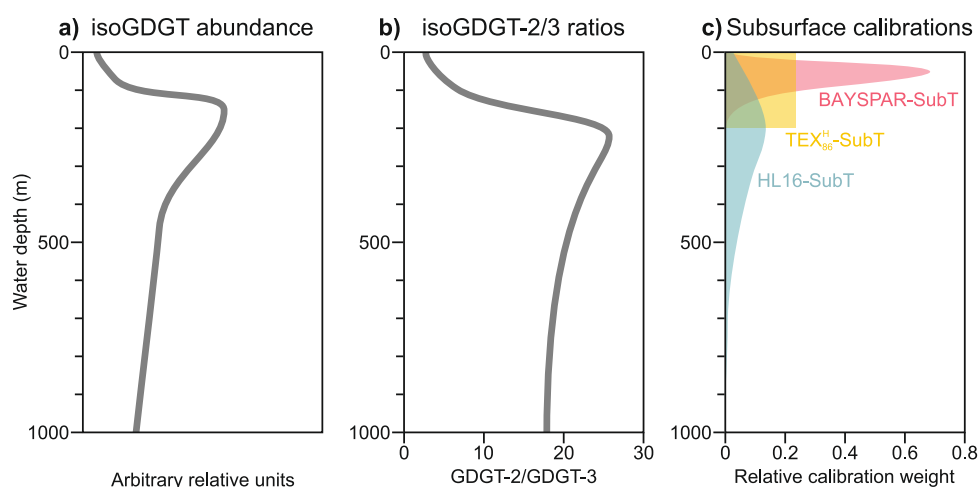


Figure 9. Conceptual figure of isoGDGT abundance (a), isoGDGT-2/3 ratios (b) and relative calibration weights (c) of three commonly used subsurface calibration models Bayspar-SubT (Tierney & Tingley, 2015), TEX₈₆^H-SubST (Kim et al., 2012b), and HL16-SubST (Ho & Laepple, 2016). Panel (c) after van der Weijst et al. (2022).

contrast, SPM-based TEX₈₆-derived temperatures are higher than in situ temperatures in shallow and deep subsurface waters where MG-I.1a and isoGDGTs are more abundant (Figure 8; Basse et al., 2014; Besseling et al., 2019; Coolen et al., 2007; Guo et al., 2024; Hernández-Sánchez et al., 2014; Hurley et al., 2018; Jia et al., 2017; Schouten et al., 2012; Spencer-Jones et al., 2021; Wittenborn et al., 2023; Wuchter et al., 2005; Xie et al., 2014). These observations could be explained by differences in seasonality (e.g., Herfort et al., 2007; Pitcher et al., 2011b), variations in export efficiency of isoGDGTs with changing water depth (e.g., Hugué et al., 2007; Wuchter et al., 2006b), and/or changes in MG-I.1a metabolic activity (Hurley et al., 2016, 2018).

Due to neutral buoyancy of single celled microorganisms, lipids (including isoGDGTs) must either be incorporated into larger particles (i.e., marine snow, fecal pellets, or phytoplankton aggregates; e.g., Hugué, Cartes, et al., 2006; Wuchter et al., 2005) or advected downward by a downwelling water mass in order to sink and become deposited at the seafloor and buried in sediments. This leads to a possible difference between the depth and timing of isoGDGT production versus export production, with the latter being recorded in the sediment. Disentangling production and export in modern systems is complicated by the timescales of modern isoGDGT measurements, where different approaches capture different time-averaged signals. SPM primarily captures a snapshot of in situ production, but may include downward flux of GDGTs in the subsurface, whereas sediment traps show seasonal and inter-annual changes in sinking particulate matter, and surface sediments can reflect years-to-several-millennia of isoGDGT accumulation and are subject to post-depositional mixing, winnowing, and/or drilling disturbance (Mekik & Anderson, 2018) and oxidation (cf. Hugué et al., 2009). Further, isoGDGTs in suspended and sinking particles may originate from a mix of both recently living and older cells and may be associated with different size fractions (Ingalls et al., 2012). Comparing data from different sample types is therefore not straightforward and understanding variations in isoGDGT production and export depth through time and across sites requires thoughtful comparison of the available data types.

Radiocarbon (¹⁴C) measurements of isolated and purified isoGDGTs or isoGDGT-derived biphytanes in sediments can indicate whether isoGDGTs originate in the near-surface or in deeper layers. In some regions (e.g., Santa Monica Basin), ¹⁴C values of isoGDGTs are lower than the local surface water dissolved inorganic carbon values, interpreted as a subsurface origin of isoGDGTs or an origin from a benthic boundary layer (Pearson et al., 2001). However, in other regions, there are no significant ¹⁴C offsets between phytoplankton lipids (e.g., alkenones) and isoGDGTs (Kusch et al., 2016; Smittenberg et al., 2004). Lateral sediment transport of pre-aged lipids (see also Section 8.6; Mollenhauer et al., 2007, 2008; Shah et al., 2008) complicates the interpretation of radiocarbon values of isoGDGTs in sediments. As a consequence, radiocarbon contents of isoGDGTs are not always a direct reflection of radiocarbon contents of dissolved inorganic carbon at the habitat, and hence export depth. Moreover, due to the analytical challenges associated with compound-specific ¹⁴C measurements, these

conclusions are based on very sparse data, and additional observations may help constrain export and lateral transport of isoGDGTs.

Variations in isoGDGT fluxes have also been related to changes in the fluxes of biogenic silica, calcite, organic carbon, chlorins and thus, net primary production (Fietz et al., 2011; Huguet et al., 2007; Mollenhauer et al., 2015; Park et al., 2018; Rice et al., 2026; Wittenborn et al., 2022; Wuchter et al., 2006b; Yamamoto et al., 2012) and recent work by Rice et al. (2026) demonstrates that increased/shallower maximum net primary production correlates positively with GDGT flux at several sites. As isoGDGT export is tied to primary production and likely relies on incorporation into larger particles (potentially due to aggregation or grazing; Huguet, Cartes, et al., 2006; Wuchter et al., 2005), export efficiency may decrease with depth of isoGDGT production. Therefore, isoGDGT export may be most efficient from surface waters even though higher isoGDGT concentrations are found in subsurface waters (Figures 8 and 9). Power law models similar to those for understanding particulate organic carbon export (Martin et al., 1987) may serve as a starting point to understand how the likelihood of export varies with depth (cf. Hurley et al., 2018; Rice et al., 2026). Such models could integrate a variety of factors, including isoGDGT abundance, TEX_{86} , and isoGDGT-2/isoGDGT-3 ratios (Figures 9a and 9b). Constraining the export depth range of the sedimentary TEX_{86} signal will help to parameterize the vertical weighting function implicit in subsurface TEX_{86} calibrations (Figure 9c) and would reduce the bias associated with applying a calibration that is systematically too shallow or too deep for the dominant GDGT export depth.

IsoGDGT concentrations in both SPM and sediment trap samples also exhibit seasonal (or sub-annual) variability. Near-surface MG-I.1a archaea are typically most active in winter, with diminished seasonality in deeper waters (Church et al., 2003; Hugoni et al., 2015; Parada & Fuhrman, 2017; Tolar et al., 2020). However, most sediment trap studies with >2 year observation periods show irregular patterns in the isoGDGT flux, with some years exhibiting a clear maximum, while other years exhibit none (Fallet et al., 2011; Huguet et al., 2007; Mollenhauer et al., 2015; Rice et al., 2026; Richey & Tierney, 2016; Turich et al., 2013; Yamamoto et al., 2012). Although peak flux generally occurs in the same season at a given site, typically the season of highest net primary production (Rice et al., 2026), sediment trap data suggest there is no globally consistent bias in isoGDGT export production to a specific season. Crucially, whilst isoGDGT concentrations can vary seasonally, TEX_{86} -based temperatures in SPM and sinking particles typically exhibit little seasonal variability (Chen et al., 2016; Fallet et al., 2011; Huguet et al., 2007; McClymont et al., 2012; Mollenhauer et al., 2015; Park et al., 2018, 2019; Rice et al., 2026; Richey & Tierney, 2016; Wittenborn et al., 2022).

6.2. Re-Evaluating Subsurface isoGDGT Production on Sedimentary isoGDGT Ratios

Most TEX_{86} estimates from sediments of Palaeogene and Cretaceous age are derived from sites with at least ~500 m water depth (Judd et al., 2022). Therefore, a deep-water (i.e., >200 m) source of isoGDGTs could bias TEX_{86} signals recorded in marine sediments and challenge the interpretation that TEX_{86} is a proxy for the temperature of the surface or shallow subsurface ocean (i.e., upper 250 m; Besseling et al., 2019; Kim et al., 2015, 2016; Taylor et al., 2013). Based on isoGDGT distributions in globally distributed surface sediments (Kim et al., 2010), Taylor et al. (2013) suggested that the isoGDGT-2/isoGDGT-3 ratio reflects the contribution of WCA MG-I.1a versus WCB MG-I.1a clades. Kim et al. (2015) demonstrated that the different isoGDGT composition of WCA and WCB (see Section 4.1 for details) can be used to trace their relative contributions to the sedimentary isoGDGT signal. This is based on the observations that in SPM and marine surface sediments collected from different regions, the isoGDGT-2/isoGDGT-3 ratio generally increases with water depth (Hernández-Sánchez et al., 2014; Kim et al., 2015, 2016; Taylor et al., 2013). This ratio is expected to increase with increasing depth and decreasing temperature in the water column due to thermal adaptation, which would increase isoGDGT-2 relative to isoGDGT-3 (e.g., Rattanasriampaipong et al., 2022; Taylor et al., 2013). However, in pure cultures of marine mesophilic *Nitrososphaeria*, temperature does not systematically affect the isoGDGT-2/isoGDGT-3 ratio (Elling et al., 2026), while the expected effect is visible when a wider range of archaea is considered (Rattanasriampaipong et al., 2022). In the currently available data sets, the observed increase in isoGDGT-2/isoGDGT-3 ratio with depth is greater than expected based on thermal adaptation alone (e.g., Rattanasriampaipong et al., 2022; Taylor et al., 2013). Generally, shallow subsurface SPM (0–200 m water depth) exhibits isoGDGT-2/isoGDGT-3 values below 5, whereas much higher values (typically ~10–25, but maxima as high as 50) are observed in deeper water. In the expanded global surface sediment data set, the correlation of isoGDGT-2/isoGDGT-3 values with water depth is weak, but statistically significant ($r = 0.54$; $p < 0.001$; Figure 10b).

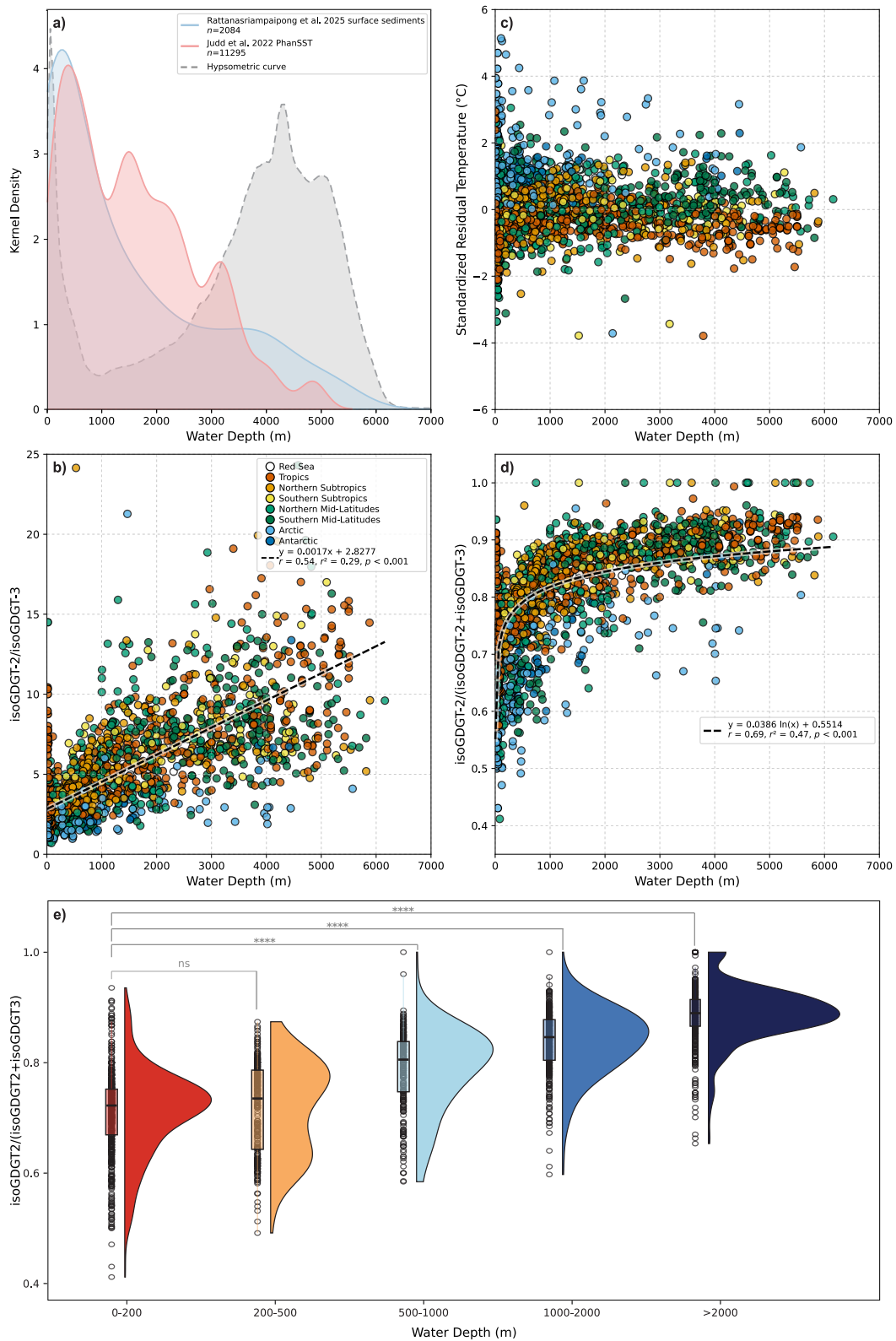


Figure 10.

However, if the fractional abundances of isoGDGT-2 and isoGDGT-3 could be used to represent the linear mixing of two end-members (WCA vs. WCB), a normalized ratio scaling from 0 to 1 would more intuitively represent the contributions of WCA versus WCB to the isoGDGT pool and would be applicable to samples where isoGDGT-3 is 0 (e.g., if isoGDGTs is below the level of detection or quantification). Therefore, we recommend using the normalized abundance of isoGDGT-2, that is, $\text{isoGDGT-2}/(\text{isoGDGT-2} + \text{isoGDGT-3})$; Behrooz et al., 2024; Rice et al., 2026), resulting in a scaling from 0 to 1 (Figure 10c). The ratio varies significantly, but on average is lower in shallow water sites with average values of 0.71 ± 0.08 (1σ) and 0.72 ± 0.08 (1σ) for sites with a water depth between 0–200 m and 200–500 m, respectively (Figures 10d and 10e). The $\text{isoGDGT-2}/(\text{isoGDGT-2} + \text{isoGDGT-3})$ ratio for these shallow water sites with 0–200 m and 200–500 m are statistically not different ($p = 0.26$). Deeper sites have higher values of 0.79 ± 0.07 (1σ), 0.84 ± 0.06 (1σ), and 0.89 ± 0.05 (1σ), respectively for water depths between 500 and 1,000 m, 1,000–2,000 m, and >2,000 m. These higher values found in the deeper sites are statistically different ($p < 0.0001$) from those found in shallow (0–200 m) water sites (Figure 10), indicating WCB contributions in deep water sites. Diminishing increases in $\text{isoGDGT-2}/(\text{isoGDGT-2} + \text{isoGDGT-3})$ at sites deeper than 500–1,000 m indicates a stabilization of WCB contributions in deeper water, potentially due to low activity of WCB and inefficient export of their biomass at depth.

Although large proportions of GDGTs from WCB—as indicated by high $\text{isoGDGT-2}/\text{isoGDGT-3}$ values—can impact TEX_{86} , changes in the fractional abundances of all other isoGDGTs included in TEX_{86} are correlated with this ratio and can lead to biases of TEX_{86} (Auderset et al., 2019; Kim et al., 2015, 2016). Given that half of all TEX_{86} paleorecords are derived from water depths below ~1,500 m, many published TEX_{86} paleotemperature records (and calibrations) likely include contributions from WCB. Indeed, 20 of 23 modern sediment trap records yield $\text{isoGDGT-2}/\text{isoGDGT-3}$ values >5 at some time of year, implying that some export of WCB-derived isoGDGTs occurs in most marine settings (Rice et al., 2026). On a regional scale, WCB contributions have been shown to bias sedimentary TEX_{86} , particularly in areas such as in the Mediterranean Sea and along the Portuguese continental margin (Kim et al., 2015, 2016). However, a study on the Chilean and Angolan continental margins found no difference in reconstructed temperatures from sediment cores obtained from different water depths, despite distinct $\text{isoGDGT-2}/\text{isoGDGT-3}$ ratios (Varma et al., 2023). On a global scale, normalized isoGDGT-2 abundances are not correlated with TEX_{86} residual temperatures in surface sediments (Figure 11b), suggesting no consistent global bias of deep water-derived isoGDGTs on TEX_{86} measured in sediments. Still, including only deep water sites from the global data set ($\geq 2,000$ m) in the surface sediment calibration, increases the correlation coefficient with SST ($r = 0.91$, $p < 0.001$; Figure 11a) compared to a calibration using only shallow sites ($r = 0.81$; Figure 11a) or the full calibration data set ($r = 0.84$, $p < 0.001$; Figure 6b). On a regional scale, alternative calibrations including only surface sediments from specific depth ranges could limit the impact of WCB contributions on TEX_{86} (Kim et al., 2015, 2016; van der Weijst et al., 2022). Similarly, individual sediment trap records indicate that WCB contributions impact TEX_{86} values of sinking particulate matter on seasonal timescales, though isoGDGT flux is biased overall to relatively higher contributions from WCA (Rice et al., 2026). Collectively, these observations indicate that contributions from WCB to sediments are less than from WCA, yet still substantial enough to be recorded in the sedimentary isoGDGT pool (Figure 10) and hence can affect TEX_{86} records. The impact of WCB on TEX_{86} varies regionally and is difficult to constrain from the relative abundance of isoGDGT-2 and isoGDGT-3, both in the modern and during past climate states.

Figure 10. (a) Water depth distribution (kernel density estimation) of modern surface sediments and the PhanSST database (estimated paleodepth) against the hypsometric curve (water depth distribution of the modern ocean based on the 15-arc s global terrain model GEBCO 2024). PhanSST data are not included in panels (b–d). (b) $\text{isoGDGT-2}/\text{isoGDGT-3}$ versus water depth in surface sediments (data source as in Figure 6). Values above 25 ($n = 3$) are not shown. (c) Standardized residual temperatures against water depth in surface sediments. (d) Normalized isoGDGT-2 abundance ($\text{isoGDGT-2}/[\text{isoGDGT-2} + \text{isoGDGT-3}]$) versus water depth in surface sediments. (e) Data visualization of all sedimentary $\text{isoGDGT-2}/[\text{isoGDGT-2} + \text{isoGDGT-3}]$ values from the global core top database, separated across a range of water depth intervals (0–200 m; 200–500 m; 500–1,000 m; 1,000–2,000 m; and >2,000 m). Box and line represent interquartile range, meaning 25th and 75th percentile as well as the median (50th percentile). Whiskers represent $1.5 \times$ interquartile range. ns = not significant. **** = p value < 0.0001. Data in panels (b–d) are colored by latitudinal bands (Arctic: $\geq 66.5^\circ\text{N}$; Antarctic: $\geq 66.5^\circ\text{S}$; Southern Mid-Latitudes: $44\text{--}66.5^\circ\text{S}$; Northern Mid-Latitudes: $40\text{--}66.5^\circ\text{N}$; Southern Subtropics: $23.5\text{--}40^\circ\text{S}$; Northern Subtropics: $23.5\text{--}40^\circ\text{N}$; Tropics: $23.5^\circ\text{S}\text{--}23.5^\circ\text{N}$; Red Sea plotted separately). Water depth for surface sediments is the modern water depth at the sampling location. Water depth for PhanSST data is the estimated paleo water depth, which was manually curated from the literature and was available for most, but not all, sites. All data are available in Elling et al. (2026).

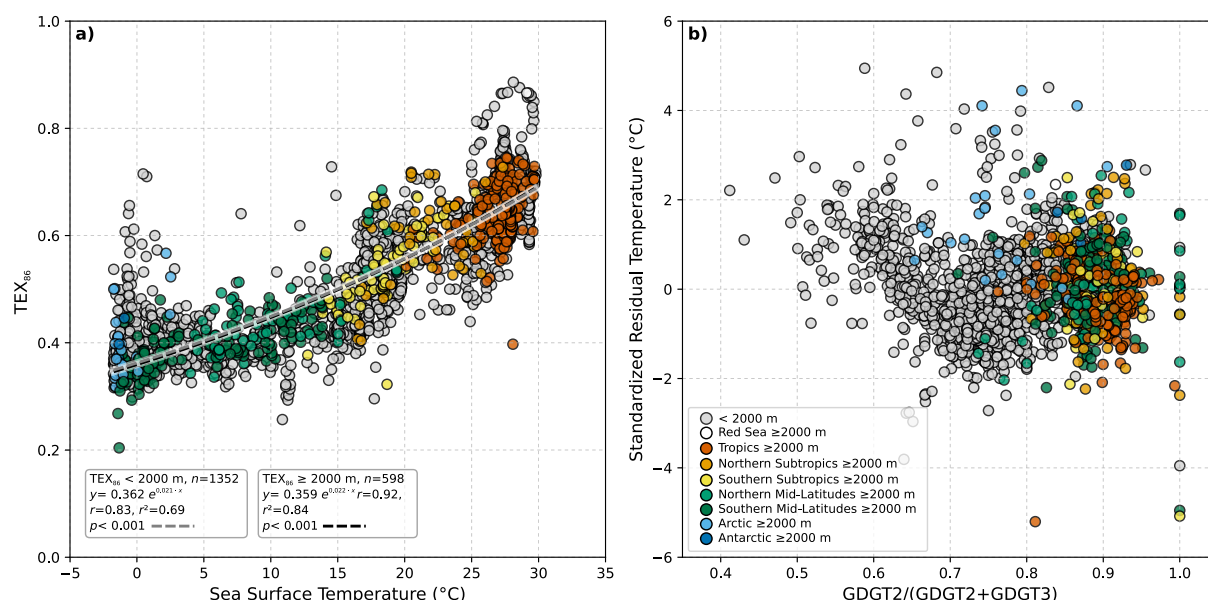


Figure 11. (a) Correlation of TEX₈₆ and sea surface temperature for surface sediments from water depths <2,000 m (gray circles and regression line) and ≥2,000 m (circles colored by latitudinal band; black regression line). (b) Standardized residual temperature (calculated using global calibrations from panel a) versus normalized isoGDGT-2 abundance (isoGDGT-2/[isoGDGT-2+isoGDGT-3]). Data from depths ≥2,000 m are colored by latitudinal bands (Arctic: ≥66.5°N; Antarctic: ≥66.5°S; Southern Mid-Latitudes: 44–66.5°S; Northern Mid-Latitudes: 40–66.5°N; Southern Subtropics: 23.5–40°S; Northern Subtropics: 23.5–40°N; Tropics: 23.5° S–23.5°N; Red Sea plotted separately). All data are available in Elling et al. (2026).

7. Influence of Physiology and Ecology of MG-I.1a *Nitrososphaeria* on the TEX₈₆-Temperature Relationship

7.1. Impact of Temperature, Salinity and Community Composition on the TEX₈₆-Temperature Relationship

The empirical correlation of temperature and TEX₈₆ in marine surface sediments is supported by experiments testing the physiological response of MG-I.1a *Nitrososphaeria* to different temperatures. Incubations of surface water in a mesocosm, resulting in an enrichment culture of a member of the MG-I.1a *Nitrososphaeria*, and subsequent growth experiments at temperatures between 5 and 35°C demonstrated that TEX₈₆ values linearly increase with growth temperature and this correlation remains linear at temperatures above 30°C (Wuchter et al., 2004). In an effort to calibrate TEX₈₆ for tropical oceans of past greenhouse climate states, Schouten et al. (2007b) performed mesocosm incubations with tropical Indian Ocean waters at temperatures between 25 and 40°C. Also in this case, a positive linear relationship was observed between temperature and TEX₈₆. However, in these early experiments, the fractional abundance of the crenarchaeol isomer was much lower than observed in marine surface sediments, hindering a direct use of these mesocosm calibrations. The reason for the low abundance of the crenarchaeol isomer is unknown, but could reflect a different archaeal source for isoGDGTs in marine sediments such as an ecotype not present in the mesocosms.

Pure cultures of *Nitrososphaeria* spp. also show a lower-than-expected relative abundance of the crenarchaeol isomer at growth temperatures up to 35°C, but there is a large increase in its abundance above this temperature in soil and thermophilic *Nitrososphaeria* spp. (compiled by Bale, Palatinszky, et al., 2019), suggesting a role of the crenarchaeol isomer in the adaptation to high temperature. When grown between 10 and 50°C, TEX₈₆ values in *Nitrososphaeria* cultures increase linearly with higher temperatures ($n = 11$; Figure 12a). This is consistent with temperature being the first-order control on the formation of cyclopentane moieties in isoGDGTs and on TEX₈₆ values. However, closely related strains of cultured *Nitrososphaeria* within the *Nitrosopumilus* cluster display species-specific variations in isoGDGT distributions (Elling et al., 2015, 2017; Pitcher et al., 2011a; Qin et al., 2015; Santoro et al., 2021; Varma et al., 2024a) and the relative abundance of IPLs and the composition of their core lipid components differ systematically between phylogenetic subgroups (Elling et al., 2017; Pitcher et al., 2011a; Schouten et al., 2008b; Varma et al., 2024a). These species-specific variations result in a relatively weak TEX₈₆-temperature relationship among cultured *Nitrososphaeria* (Figure 12a) and suggest that changes in

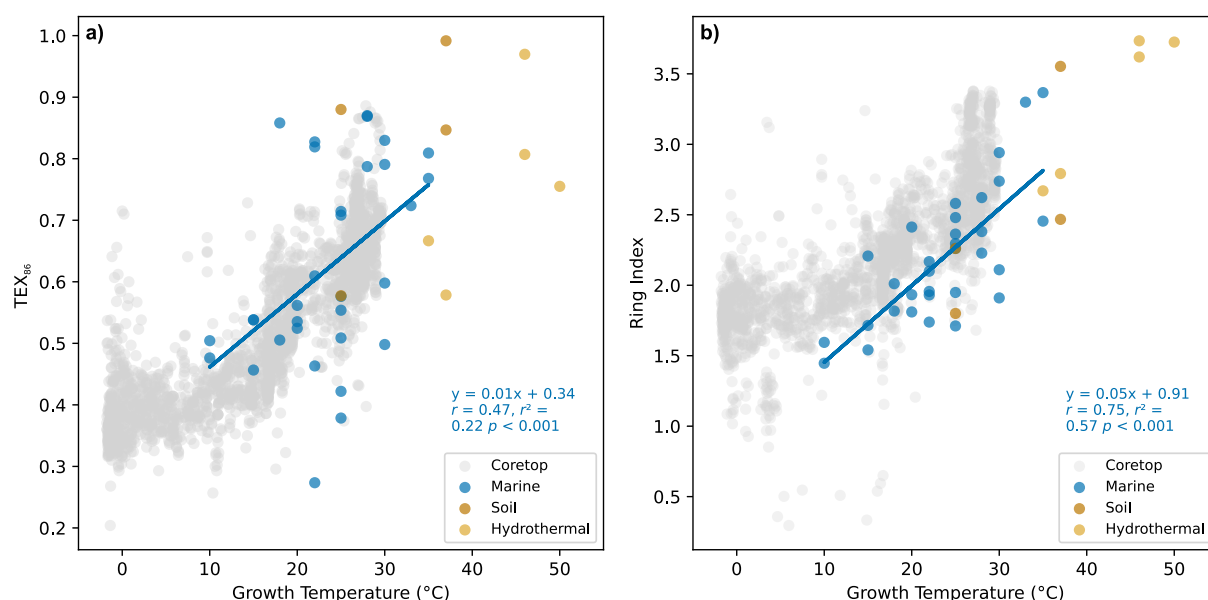


Figure 12. Empirical relationship between (a) TEX₈₆ (Schouten et al., 2002) and (b) Ring Index (following the definition of Zhang et al., 2016) with growth temperature in *Nitrososphaeria* culture data (Bale, Palatinszky, et al., 2019; Elling, 2015; Elling et al., 2014, 2015, 2017; Pitcher et al., 2011a; Qin et al., 2015; Sinninghe Damsté et al., 2012b). Regression lines only include marine MG-I.1a (blue circles). For reference, global surface sediment data (gray circles; as in Figure 6; Rattanasriampaipong et al., 2025) as well as soil (brown circles) and hydrothermal (yellow circles) *Nitrososphaeria* from the lineage HWCG, SAGMCG, and I.1b are also shown. All data are available in Elling et al. (2026).

community composition could lead to distinct TEX₈₆-temperature relationships (Elling et al., 2015). Changing community composition could be responsible for the spatially-varying TEX₈₆-temperature relationships observed in global surface sediments (Figure 6). This may be particularly relevant in restricted basins such as the Mediterranean Sea and Red Sea, and brackish environments such as the Black Sea and Baltic Sea, which host endemic populations of *Nitrososphaeria* (Ionescu et al., 2009; Labrenz et al., 2010; Qian et al., 2011; Wittenborn et al., 2023). Such endemic communities may also explain why these environments feature distinct isoGDGT fingerprints, such as low abundances of the crenarchaeol isomer and high abundances of OH-isoGDGTs observed in the Baltic Sea (Kabel et al., 2012; Kaiser & Arz, 2016).

Spatial and temporal shifts in archaeal community composition, resulting in changing TEX₈₆-temperature relationships, have been suggested for the modern Red Sea (Trommer et al., 2009). In the geological record, shifts in community composition have been suggested as explanations for anomalous isoGDGT distributions in the Early Cretaceous proto-North Atlantic (~137–125 Ma; Littler et al., 2014), the early Eocene SW Pacific (~56–48 Ma; Inglis et al., 2015a), the Plio-Pleistocene Mediterranean Sea (~3–0.8 Ma; Polik et al., 2018), and the Quaternary Iberian Margin (70–0 ka; Darfeuil et al., 2016). Changes in community composition may not only be driven by geographic isolation but also by changes in physicochemical parameters such as strong changes in salinity and pH. Although these factors do not impact TEX₈₆ in cultures and mesocosms (Elling et al., 2015; Wuchter et al., 2004), strong variations in these parameters such as in marginal brackish seas may select for specifically adapted species with distinct physiology and TEX₈₆-temperature relationships (Elling et al., 2015; Sinninghe Damsté et al., 2022).

The global TEX₈₆-RI relationship has been used to identify anomalous isoGDGT distributions in sediments that may be affected by non-thermal effects (see Section 8; Zhang et al., 2016), including community composition (Polik et al., 2018). The Ring Index (RI) is correlated to (a) TEX₈₆ and (b) SST in mesocosms and global surface sediments (Schouten et al., 2002; Wuchter et al., 2004; Zhang et al., 2016). Here the RI is defined following Zhang et al. (2016):

$$RI = \frac{[\text{isoGDGT} - 0] + [\text{isoGDGT} - 1] + 2 \times [\text{isoGDGT} - 2] + 3 \times [\text{isoGDGT} - 3] + 4 \times [\text{crenarchaeol}] + 4 \times [\text{crenarchaeol isomer}]}{[\text{isoGDGT} - 0] + [\text{isoGDGT} - 1] + [\text{isoGDGT} - 2] + [\text{isoGDGT} - 3] + [\text{crenarchaeol}] + [\text{crenarchaeol isomer}]} \quad (7)$$

This version of the RI multiplies crenarchaeol (and its isomer) by a factor of four and hence does not take into account the presence of the additional cyclohexane moiety, ignoring the unique effect the cyclohexane moiety has on the physical properties of an isoGDGT membrane (Sinninghe Damsté et al., 2002). The latter introduces a “bulge” into its 3D structure, preventing dense packing of isoGDGTs (Sinninghe Damsté et al., 2002), and its inclusion would thus be expected to weaken rather than strengthen the RI–SST relationship. However, increases of RI in *Nitrososphaeria* at higher temperatures are driven by higher fractional abundances of crenarchaeol and its isomer, suggesting that it is involved in adaptation to higher temperature (e.g., Bale, Palatinszky, et al., 2019; Elling et al., 2015; Qin et al., 2015; Sinninghe Damsté et al., 2018). In pure culture experiments, the relationship between the RI and growth temperature is statistically stronger ($r = 0.75$, $p = 6.8 \times 10^{-7}$; Figure 12b) than the relationship between TEX₈₆ and growth temperature ($r = 0.47$, $p = 0.007$; Figure 12a). This may be related to different sensitivities of isoGDGT-1, isoGDGT-2 and isoGDGT-3 to non-temperature effects in culture experiments and/or the low abundance of the crenarchaeol isomer in all currently available cultures (Elling et al., 2015; Pitcher et al., 2011a; Qin et al., 2015). Although both TEX₈₆ and RI show robust relationships with growth temperature in culture experiments, temperature is not the sole control and other non-thermal influences are likely to be important (see Section 7.2 below).

7.2. Impact of Metabolic Activity of *Nitrososphaeria* on TEX₈₆

The TEX₈₆ proxy is interpreted to mainly reflect changes in ocean temperatures. However, archaeal membrane lipid distributions can also be influenced by other physiological and environmental controls, potentially influencing paleo-SST estimates. For example, in *Nitrososphaeria* cultures the number of cyclopentane moieties in isoGDGT is inversely correlated with substrate availability, either in the form of the electron donor (NH₃; Elling et al., 2014; Evans et al., 2019; Hurley et al., 2016) or the electron acceptor (O₂; Qin et al., 2015). Faster ammonia oxidation rates are associated with lower TEX₈₆-derived temperatures, while limited substrate availability and slower ammonia oxidation rates are associated with higher TEX₈₆-derived temperatures. This effect is thought to derive from reduced proton permeability of cellular membranes with a higher degree of isoGDGT cyclization that promotes energy conservation and increasing growth efficiency at low substrate availability (Hurley et al., 2016), an effect, that is, also observed in cultures of other archaea (Quehenberger et al., 2020; Zhou et al., 2020).

The dependence of TEX₈₆ on ammonia oxidation rate in cultures is mechanistically consistent with offsets observed between in situ temperatures and TEX₈₆-derived temperatures in SPM (e.g., Hurley et al., 2018; Wuchter et al., 2005; Zhu et al., 2016). In high productivity locations, with presumably higher nitrification (and hence ammonia oxidation) rates due to elevated remineralization rates, such as the Eastern Tropical North Pacific, TEX₈₆-derived temperatures in SPM are lower than in situ temperatures by up to 25°C (Figure 8; Xie et al., 2014). In both eutrophic (nutrient-rich) and oligotrophic (nutrient-poor) sites, the lowest TEX₈₆ values in SPM are often observed at water depths where ammonia oxidation rates and/or nitrite concentrations (the product of ammonia oxidation) are highest (Hurley et al., 2016, 2018). This is presumably due to higher ammonia oxidation rates near the base of the euphotic zone where ammonia is supplied from organic matter remineralization (Hurley et al., 2016, 2018). Conversely, TEX₈₆-derived temperatures higher than in situ temperatures are observed in SPM below the base of the euphotic zone of oxic water columns (Figure 8; e.g., Hernández-Sánchez et al., 2014; Hurley et al., 2018; Turich et al., 2007; Wuchter et al., 2005) and align with generally lower ammonia oxidation rates in this zone (Hurley et al., 2016, 2018). These trends are observed independently of particle size class, and therefore may represent in situ adaptive responses of *Nitrososphaeria* rather than a signal derived from admixture of SPM exported from warmer surface waters (Hurley et al., 2018).

However, it remains unclear how such metabolic effects are reflected in global surface sediments calibrations and paleorecords. Due to the diverse nutrient regimes covered by the global surface sediment data sets, physiological factors and changing ammonia oxidation rates may explain some of the non-temperature variability in global TEX₈₆-temperature regressions. Further, it remains to be tested whether the global calibration data sets are biased

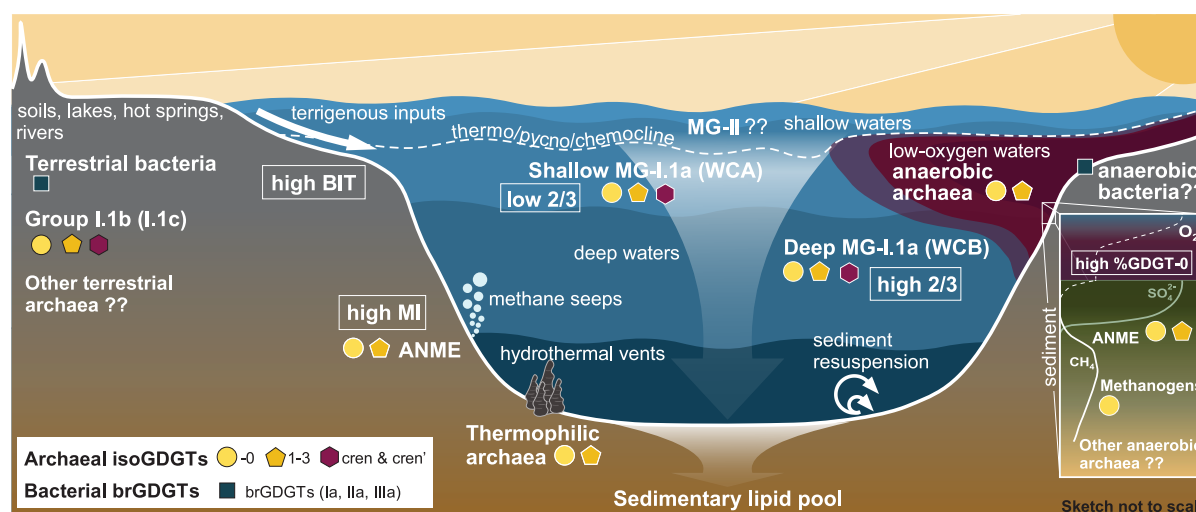


Figure 13. Sources of archaeal lipids contributing to the sedimentary lipid pool in the ocean. Also shown are sources of bacterial brGDGTs that are commonly used alongside archaeal lipid-based proxies. ANME: Anaerobic methanotrophic archaea; MG-I: Marine Group I *Nitrososphaeria*; MG-II: Marine Group II *Euryarchaeota*; 2/3: isoGDGT-2/isoGDGT-3 ratio; BIT: Branched and Isoprenoid Tetraether index; MI: Methane Index; WCA: Water Column Group A; WCB: Water Column Group B.

towards specific nutrient regimes or whether they broadly reflect diverse nutrient regimes. To this end, Rattanapong et al. (2025) suggested that an effect of the nutrient regime is preserved in sedimentary TEX_{86} records and can be detected after accounting for the thermal signal in global surface sediment data sets, providing an alternative explanation for anomalous TEX_{86} values in surface sediments such as from the Red Sea.

Anomalous isoGDGT distributions are also observed during past nitrogen cycle perturbations such as during the Oceanic Anoxic Events of the Cretaceous (~94–86 Ma; Junium et al., 2018) or during sapropel formation in the Mediterranean Sea in the Pliocene and Pleistocene (3–0.8 Ma; Menzel et al., 2006; Polik et al., 2018). In the Mediterranean Sea, TEX_{86} -reconstructed temperatures during the Pliocene and Pleistocene can vary by up to 20°C, which is implausible given the background climate and other independent proxy records (Menzel et al., 2006; Polik et al., 2018). Instead, the variations may be related to either (a) a change in habitat depth due to expansion of euxinia and/or (b) changes in nutrient supply in response to nitrogen cycle perturbation (Menzel et al., 2006; Obrecht et al., 2025; Polik et al., 2018). Similarly, changes in TEX_{86} and isoGDGT distributions towards lower reconstructed temperatures may be related to increased nutrient supply during enhanced upwelling (Alfken et al., 2020; Rommerskirchen et al., 2011). This mechanism has been invoked to explain anomalously low TEX_{86} values in sediments of Miocene-Pliocene age from the eastern Equatorial and southwest Pacific (~6–3 Ma; Grant et al., 2023; Lawrence et al., 2020), sediments of Miocene-Pliocene age from the southeast South Atlantic (~14–3 Ma; Rommerskirchen et al., 2011), and sediments of late Eocene age from the eastern tropical Atlantic (~38–34 Ma; Cramwinckel et al., 2018). However, whether lower-than-expected TEX_{86} values record changes in (a) metabolic activity, (b) a shift in habitat depth towards colder waters, and/or (c) changes in thermal structure (thermocline depth, upwelling of cold water) remains to be shown.

8. Additional Sources of isoGDGTs in the Marine Environment

The sedimentary isoGDGT pool in most marine settings is dominated by input from planktonic MG-I.1a *Nitrososphaeria* (see Sections 4–7). However, there are other potential sources of isoGDGTs in the marine environment that may overprint TEX_{86} values recorded in sediments. Below we discuss these additional sources and the extent to which they control the interpretation of paleo-SST reconstructions.

8.1. Input of isoGDGTs by Methanogenic Archaea

Methanogenic archaea (methanogens) from two notable phyla—*Methanobacteriota* and *Halobacteriota* (Syn. class-level lineages within *Euryarchaeota*; see Table 1)—are known to biosynthesize isoGDGTs (Zeng et al., 2022, and references therein) and are abundant in anoxic marine sediments and/or the water column (Figure 13). Methanogens characteristically biosynthesize archaeols and isoGDGTs with a high relative

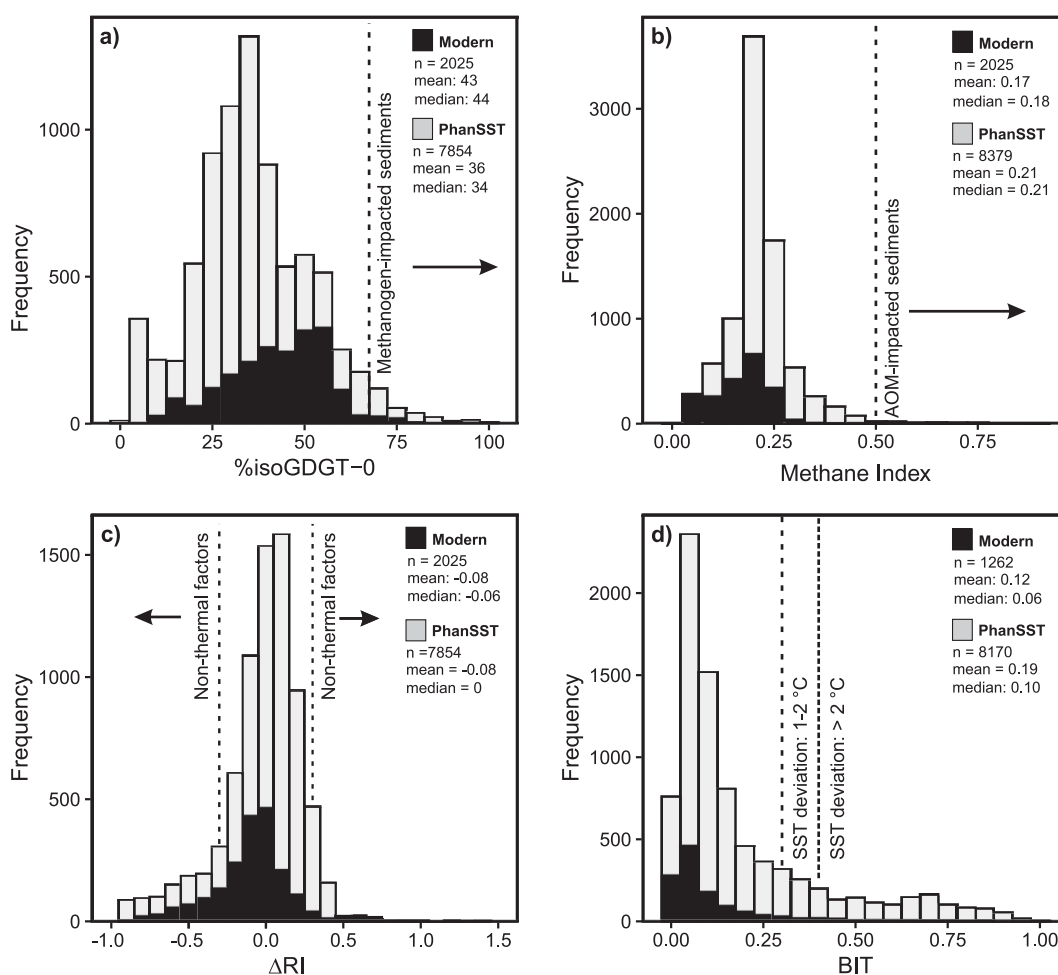


Figure 14. Histogram of (a) %isoGDGT-0 values, (b) Methane Index (MI), (c) delta Ring Index (Δ RI) and (d) BIT index from modern marine surface sediments (black; for data sources see Figure 6) and Mesozoic and Cenozoic marine sediments (gray; Judd et al., 2022 and references therein). These data are compiled from a large number of independent studies that may be subject to various sampling biases, including avoiding surface sediments that may be subject to non-thermal overprints, such as those from near river mouths or in areas impacted by methane cycling. Although the data may not be fully representative of global marine sediments, it does encompass all data used for global core-top calibrations and paleotemperature studies.

proportion of isoGDGT-0 (De Rosa & Gambacorta, 1988; Koga et al., 1993b). Thus, the ratio of isoGDGT-0 versus crenarchaeol (isoGDGT-0/cren), originally proposed by Blaga et al. (2009), and the modified %isoGDGT-0 index (expressed as $[\text{isoGDGT-0}] / ([\text{isoGDGT-0}] + [\text{Cren}]) \times 100$; Inglis et al., 2015b; Sinninghe Damsté et al., 2012a) are used to identify a high relative contribution of methanogens to the isoGDGT pool in marine sediments. Pure and enrichment cultures belonging to the family *Nitrosopumilaceae* yield isoGDGT-0/cren values <2 and %isoGDGT-0 values <67%, such that an additional, potentially methanogenic, source of isoGDGT-0 is likely when values exceed these thresholds (Blaga et al., 2009; Inglis et al., 2015b; Naeher et al., 2014; Sinninghe Damsté et al., 2012a). In open ocean sediments, methanogenic contributions are thought to be relatively minor (Inglis et al., 2015b), whereas in marginal marine settings (where terrigenous input can be high) and/or sites characterized by active methane cycling (e.g., cold seeps), methanogenic contributions can be significant (Aloisi et al., 2002; Pancost & Sinninghe Damsté, 2003; Weijers et al., 2011). However, as most known mesophilic methanogens do not biosynthesize isoGDGTs with cyclopentane moieties (reviewed in De Rosa & Gambacorta, 1988; Koga et al., 1993b; Schouten et al., 2013b), the impact of methanogenesis on sedimentary TEX_{86} values (but potentially not RI) may be low and the median %isoGDGT-0 index value in modern surface sediments (44%; Figure 14a) and Mesozoic-to-Cenozoic (~190 Ma to present) sediments (34%; Figure 14a) suggests overall limited impact of methanogens on the published paleo-reconstructions.

As isoGDGT-0 is also biosynthesized by a diverse range of non-methanogenic archaea (see Section 2), it is unclear whether high isoGDGT-0/cen values truly reflect a contribution from methanogenic archaea. Further, no empirical study has so far been published that directly relates the abundance (e.g., through DNA-based methods) of methanogens or other archaea to isoGDGT-0 abundance. Carbon isotopic analysis has however been used to provide insights into the sources of sedimentary isoGDGT-0. If isoGDGT-0 is predominantly derived from MG-I.1a *Nitrososphaeria*, the stable carbon isotopic composition ($\delta^{13}\text{C}$) of isoGDGT-0 should be identical or similar to that of crenarchaeol (Pancost et al., 2008; Pearson et al., 2016; Polik et al., 2018; Schouten et al., 1998), whereas deviations indicate a different source of these two compounds and hence a contribution from heterotrophic, methanogenic, or methanotrophic benthic archaea. Although the overall data set is currently limited, the consistently lower $\delta^{13}\text{C}$ values of isoGDGT-0 compared to crenarchaeol in modern open ocean sediments suggest contributions from archaea other than MG-I.1a to the sedimentary isoGDGT-0 pool (Pearson et al., 2016; Zhu et al., 2021), justifying its exclusion from TEX_{86} .

8.2. Input of isoGDGTs via Anaerobic Methanotrophs and Alkanotrophs

Anaerobic methane-oxidizing (ANME) archaea are phylogenetically related to methanogens and thrive in anoxic water columns and marine sediments with high methane concentrations, such as cold seeps (for reviews see Knittel & Boetius, 2009; Wegener et al., 2022). In consortia with sulfate-reducing bacteria, ANME archaea are responsible for the anaerobic oxidation of methane, a process that is a major sink of methane in marine sediments (Boetius et al., 2000; Hinrichs et al., 1999; Reeburgh, 1982). To date, three distinct ANME archaeal clusters, namely ANME-1, ANME-2, and ANME-3, are assigned within order-level lineages of the phylum *Halobacteriota*. Only ANME-1 archaea are known to biosynthesize isoGDGTs (with the exception of the ANME-2c and ANME 2d sub-clusters; Kurth et al., 2019; Niemann & Elvert, 2008, and references therein). ANME-1 archaea predominantly biosynthesize isoGDGT-1 to -4 (Aloisi et al., 2002; Blumenberg et al., 2004; Pancost et al., 2001; Rossel et al., 2008, 2011; Thiel et al., 2007). However, in hydrothermally influenced sediments, ANME archaea predominantly produce isoGDGT-4 (Kellermann et al., 2016; Schouten et al., 2003a). A polyphyletic group of so-called anaerobic multicarbon alkane-degrading archaea (ANKA) related to known ANME archaeal lineages (Wegener et al., 2022) suggest widespread capacity to produce isoGDGT-0, but only one species was found to produce isoGDGTs with cyclopentane moieties, specifically isoGDGT-1 and isoGDGT-2 (Zehnle, 2023).

ANME archaea are particularly abundant in the deep euxinic waters of the Black Sea. This was originally inferred via the occurrence of ^{13}C -depleted biphytanes, derived from isoGDGTs (Schouten et al., 2001; Wakeham et al., 2003; Zhu et al., 2024) and the high relative abundance of isoGDGT-2 (equal to isoGDGT-0) in particulate organic carbon (POC) collected from water depths >1,000 m. 16S rRNA sequencing later revealed that the Black Sea archaeal community is dominated by *Nitrososphaeria* in the upper water column (<105 m) but that the deep sulfidic waters (>110 m) are dominated by diverse archaeal communities, including those belonging to ANME-1b (e.g., Coolen et al., 2007; Lam et al., 2007; Schubert et al., 2006; Sollai et al., 2019a). Given the significant positive correlation ($r > 0.99$) between ANME-1b archaeal gene reads and IPL-isoGDGT-0 to IPL-isoGDGT-2, it is highly probable that ANME-1b archaea biosynthesize these isoGDGTs in the Black Sea (Sollai et al., 2019a). Intriguingly, there is an absence of ^{13}C -depleted biphytanes and ANME-type isoGDGT distributions in Black Sea sediments. This implies that the water column ANME archaeal signal is not effectively transferred into the sedimentary record (Schouten et al., 2001; Wakeham et al., 2003) and may explain why the presence of ANME biomarkers has only rarely been observed in the geological record outside of cold seep areas (e.g., Kim & Zhang, 2022; Wang et al., 2023).

In contrast to planktonic ANME archaea, benthic ANME archaea and ANKA likely contribute to the sedimentary isoGDGT records in areas with intensive sedimentary methane cycling (Figure 13). In such settings, significant isoGDGT contributions by these archaea have been observed both in the modern (e.g., Keller et al., 2025b; Schouten et al., 2003a; Zhang et al., 2011) and geologic record (e.g., Birgel et al., 2008; Kim & Zhang, 2022), potentially skewing TEX_{86} estimates from these areas (e.g., Ho et al., 2025; Keller et al., 2025b; Zhang et al., 2011). The contribution of ANME archaea to marine sediments can be evaluated using isoGDGT ratios such as the isoGDGT-2/cenarchaeol ratio (Weijers et al., 2011) or via the “Methane Index” (MI; Zhang et al., 2011), a proxy that evaluates the relative contribution of methanotrophic archaea (represented by elevated isoGDGT-1, isoGDGT-2 and isoGDGT-3) versus MG-I.1a *Nitrososphaeria* (represented by elevated cenarchaeol and its isomer):

$$MI = \frac{[isoGDGT - 1] + [isoGDGT - 2] + [isoGDGT - 3]}{[isoGDGT - 1] + [isoGDGT - 2] + [isoGDGT - 3] + [crenarchaeol] + [crenarchaeol isomer]} \quad (8)$$

High MI values (>0.3–0.5) indicate enhanced contribution from anaerobic methanotrophs to the sedimentary isoGDGT pool (Kim & Zhang, 2023; Zhang et al., 2011). The median MI value in modern surface sediments (0.18; Figure 14b) and Mesozoic-to-Cenozoic sediments (0.21; Figure 14b) suggests limited ANME archaea overprints in published paleotemperature records and the global surface sediment calibrations. The MI has been employed to reconstruct anaerobic methanotrophic activity and high MI values provide evidence for enhanced methane oxidation in the Northern Cascadia Margin during the Late Glacial (~20 ka; Kim & Zhang, 2023) and across the Eocene to Miocene sedimentary succession of the North Atlantic (43–18 Ma; Wang et al., 2023), and the SW Pacific Ocean during the Oligocene/Miocene transition (23 Ma; Kim & Zhang, 2022). TEX₈₆ values may already be biased by contributions from ANME archaea below the MI threshold of 0.3–0.5 (Keller et al., 2025b). Conversely, when MI values exceed 0.3, the bias on TEX₈₆-derived temperatures may not always be as significant as assumed (Ho et al., 2025). Further, since not all ANME subgroups produce isoGDGTs with cyclopentane moieties, low MI values do not necessarily indicate the absence of ANME archaea. Therefore, the use of the MI to reconstruct past changes in sedimentary methane cycling may be more reliable when combined with other biomarkers and/or the occurrence of a ¹³C-depleted isotopic signature (e.g., archaeol, isoGDGTs, or isoGDGT-derived biphytanes; Hinrichs et al., 1999; Naeher et al., 2014; Pancost et al., 2001; Schouten et al., 2003a; Zhang et al., 2011).

The ΔRI (Zhang et al., 2016) complements the MI and describes a sample's offset between its RI and its RI_{TEX} (ΔRI = RI_{TEX}–RI), with RI_{TEX} representing the expected RI based on the sample's TEX₈₆ value and a quadratic regression of RI with TEX₈₆ in modern surface sediments (Zhang et al., 2016):

$$RI_{TEX} = -0.77 \times TEX_{86} + 3.32 \times (TEX_{86})^2 + 1.59 \quad (9)$$

Marine sediments with a ΔRI value between +0.3 and –0.3 are generally considered robust for temperature reconstructions (Zhang et al., 2011). For sediments that lie outside this range, the sedimentary isoGDGT content is likely impacted by non-thermal factors, including (but not limited to) the contribution from ANME archaea (Zhang et al., 2016). In modern and deep-time marine sediments used for temperature reconstructions (Figure 14c), the median ΔRI value falls within this range (–0.06 and 0, respectively) and indicates that the impact of these non-thermal overprints are generally minor in most settings.

8.3. Input of isoGDGTs via Benthic Non-Methane Cycling Archaea

Besides methanogenic and methanotrophic archaea, sediments host diverse communities of uncultured benthic archaea with other metabolic strategies, such as benthic *Nitrososphaeria* and heterotrophic archaea from diverse lineages (Baker et al., 2020). These benthic archaea could represent a source of isoGDGTs to marine sediments (Biddle et al., 2006), and this could bias TEX₈₆ records (Lengger et al., 2012; Lipp & Hinrichs, 2009; Liu et al., 2011; Xiao et al., 2023b). For example, input of OH-isoGDGT-0 from benthic *Nitrososphaeria* was suggested to occur in hadal trench sediments, inducing a cold bias in OH-isoGDGT-based proxies (Xiao et al., 2023b). However, labeling experiments suggest a low activity of aerobic benthic *Nitrososphaeria* in marine sediments (Lengger et al., 2014b) and in open marine sediments and methane seep sediments, isoGDGT δ¹³C values suggest that heterotrophic benthic archaea make minimal contributions to the isoGDGT pool (Keller et al., 2025b; Pearson et al., 2016; Zhu et al., 2021). Furthermore, by studying core lipid and IPL-isoGDGTs in Arabian Sea sediments below the OMZ, Lengger et al. (2012) showed that: (a) benthic isoGDGT lipids were more susceptible to degradation than fossil isoGDGTs and (b) that benthic IPL-isoGDGTs did not provide a significant contribution to core lipid isoGDGTs and, hence, did not affect TEX₈₆ values. Similarly, IPL- and core-isoGDGT δ¹³C values in Black Sea sediments confirm that anaerobic benthic archaea are unlikely to be a major contribution to the pool of isoGDGTs with cyclopentane moieties, although they may contribute to the isoGDGT-0 pool (Schouten et al., 2001; Wakeham et al., 2003; Zhu et al., 2024).

Bathyarchaeia are also considered as a source of isoGDGTs. *Bathyarchaeia* are abundant in anoxic subsurface and marine sediment environments, where they are thought to play important roles in the degradation of diverse organic matter substrates (Hou et al., 2023). *Bathyarchaeia* abundance correlates with isoGDGT concentrations

in sediments (Besseling et al., 2018; Meador et al., 2015) and the only described enrichment culture of *Bathyarchaea* produces isoGDGTs with up to three cyclopentyl moieties (Dong et al., 2025).

In addition, in estuarine sediments the $\delta^{13}\text{C}$ signature of isoGDGTs is lower than expected when assuming input from planktonic *Nitrososphaeria* alone (Meador et al., 2015). Analysis of archaeal viruses in sediments also suggests a high turnover of the benthic archaeal community, resulting in the accumulation of archaeal necromass (Danovaro et al., 2016), potentially including isoGDGTs. Benthic archaea may also recycle isoGDGTs as an adaptation to low-energy availability (Takano et al., 2010). However, it remains to be shown how prevalent this process is and whether recycling exerts an effect on TEX_{86} .

In summary, the contrasting lines of evidence indicate a need for further studies to assess whether benthic isoGDGT production can significantly bias sedimentary TEX_{86} values. This could potentially be assessed by analyzing biomarkers specific to benthic archaea such as isoBDGTs and isoPDGTs (Coffinet et al., 2020; Dong et al., 2025).

8.4. Hydrothermal Input and Degradation of isoGDGTs

Diverse and abundant (non-*Nitrososphaeria*) archaea inhabit marine hydrothermal vents and plumes as well as proximal sediments (Takai & Nakamura, 2011; Zhou et al., 2022). Archaea inhabiting hydrothermal systems experience drastically different environmental conditions (e.g., temperature, pH) than those that inhabit mesophilic marine environments. As such, their lipid composition and adaptation mechanisms differ strongly from those of mesophilic archaea (e.g., Gibson et al., 2013; Lincoln et al., 2013; Pan et al., 2016; Sollich et al., 2017). These extremophilic archaeal communities typically produce a distinct biomarker distribution that contains isoGDGTs and isoGMGTs with up to eight rings, among other lipids (Gibson et al., 2013; Jaeschke et al., 2012, 2014; Lincoln et al., 2013; Liu et al., 2016; Pan et al., 2016, 2016, 2016; Schouten et al., 2003a; Sollich et al., 2017; Umoh et al., 2020). Input of isoGDGTs derived from hydrothermal systems could thus influence sedimentary isoGDGT distributions and bias isoGDGT-derived proxies, including TEX_{86} . Anomalous isoGDGT distributions have been found in and near hydrothermal vents and in hydrothermally heated sediments, yielding unrealistic TEX_{86} values and distinct offsets from the TEX_{86} -RI relationship of marine background sediments (e.g., Lincoln et al., 2013; Pan et al., 2016). Besides the distinct isoGDGT composition of thermophilic archaea (e.g., Lincoln et al., 2013; Pan et al., 2016; Schouten et al., 2003a), anomalous TEX_{86} values in hydrothermal systems have been attributed to the impact of differential diagenetic and catagenetic degradation of cyclized isoGDGTs in hydrothermally heated sediments (Bentley et al., 2022; see also Section 9). This influence of hydrothermal communities and catagenetic processes on sedimentary isoGDGT distributions diminishes with decreasing temperature of hydrothermally heated sediments and increasing distance from the hydrothermal vents due to dilution by the isoGDGT flux from mesophilic archaea (e.g., Bentley et al., 2022; Schouten et al., 2003a; Sollich et al., 2017; Umoh et al., 2020). Evidence from a range of hydrothermal systems has further shown that the effect of isoGDGT input or degradation may vary on a site-by-site basis (e.g., Bentley et al., 2022; Hu et al., 2012; Pan et al., 2016; Umoh et al., 2020). A significant contribution from hydrothermal input may be identified by other geochemical hydrothermal vent plume indicators (e.g., Pan et al., 2016), as well as specific isoGDGT distributions, such as increased fractional abundances of isoGDGT-1 through isoGDGT-3 (and therefore higher MI) and/or the high relative abundance of cyclized isoGMGTs (e.g., Jaeschke et al., 2014; Pan et al., 2016; Schouten et al., 2003a; Sollich et al., 2017). Overall, this bias is likely only important very close to hydrothermal vents.

8.5. Terrigenous Input of isoGDGTs

While Group I.1a *Nitrososphaeria* predominate in mesophilic marine waters and sediments, other *Nitrososphaeria* as well as other archaea living in lakes, rivers, soils, and peats can produce a similar suite of isoGDGTs (e.g., Blaga et al., 2009; Elling et al., 2017; Kim et al., 2007; Naafs et al., 2018; Sinninghe Damsté et al., 2012b). Inputs of these allochthonous (terrigenous) lipids to marine sediments could alter the primary marine signals and bias reconstructed TEX_{86} temperatures (Herfort et al., 2006; Weijers et al., 2006). A way of tracing terrigenous isoGDGTs is by comparing the abundance of isoGDGT relative to those of branched GDGTs (brGDGTs). BrGDGTs, synthesized by *Acidobacteria* and potentially other bacteria (Chen et al., 2022, 2025; Halamka et al., 2021, 2023; Sinninghe Damsté et al., 2011), vary in the number of methyl branches and cyclopentane moieties. They are typically much more abundant in the terrestrial environment (Weijers et al., 2007), although relatively low amounts of brGDGTs (~1–2 orders of magnitude lower than co-occurring isoGDGTs) can also be produced in situ in marine surface sediments and the water column (e.g., Hopmans et al., 2004; Liu

et al., 2014; Peterse et al., 2009; Schmidt et al., 2010; Sinninghe Damsté, 2016; Xiao et al., 2026; Xie et al., 2014; Zell et al., 2014). The branched versus isoprenoid tetraether index (BIT) was developed to trace terrigenous input into marine sediments and is defined as (De Jonge et al., 2014; Hopmans et al., 2004):

$$\text{BIT} = \frac{[\text{brGDGT} - \text{Ia}] + [\text{brGDGT} - \text{IIa}] + [\text{brGDGT} - \text{IIa}'] + [\text{brGDGT} - \text{IIIa}] + [\text{brGDGT} - \text{IIIa}']}{[\text{brGDGT} - \text{Ia}] + [\text{brGDGT} - \text{IIa}] + [\text{brGDGT} - \text{IIa}'] + [\text{brGDGT} - \text{IIIa}] + [\text{brGDGT} - \text{IIIa}'] + [\text{crenarchaeol}]} \quad (10)$$

where brGDGT-X describes brGDGTs with 4–6 methyl groups in roman numerals and prime symbol (') indicates the 6-methyl isomer(s). BIT ranges from 0 to 1 and evaluates the relative input of predominantly terrigenous brGDGTs versus marine-derived crenarchaeol. Although allochthonous brGDGTs can reach remote ocean environments via aeolian transport (Fietz et al., 2013), low BIT values are typically observed in sediments from the open ocean (low terrigenous inputs), whereas higher BIT values are observed in coastal marine sediments, close to river deltas (e.g., Hopmans et al., 2004; Schmidt et al., 2010; Sinninghe Damsté, 2016; Zell et al., 2014). Early work, therefore, suggested that marine sediments with BIT values >0.4 should not be used for TEX₈₆ temperature reconstructions, as above this threshold the error introduced by input of terrigenous isoGDGTs becomes larger than the analytical error of TEX₈₆ (Weijers et al., 2006). However, this threshold is specific to a single depositional system (the Congo Fan), and the impact of terrigenous isoGDGTs on reconstructed SST will depend on the composition of isoGDGTs in the surrounding (terrestrial) catchment.

The median BIT index value in modern surface sediments (0.06; Figure 14d) and Mesozoic-to-Cenozoic sediments (0.10; Figure 14d) implies that marine sediments used for the global surface sediment calibrations and global paleoclimate compilations are largely unaffected by substantial terrigenous overprinting of isoGDGTs. However, compound-specific $\delta^{13}\text{C}$ analysis of isoGDGT-derived biphytanes shows that terrigenous isoGDGTs can bias TEX₈₆ values even when BIT values are <0.3 (Pearson et al., 2016; Zhu et al., 2021). Subsequent studies show that the BIT threshold for excluding TEX₈₆ values varies on a site-by-site basis. For example, Quaternary-aged sediments from the northwestern Mediterranean are characterized by low BIT values (<0.4), suggesting a minor impact on TEX₈₆ SST estimates. However, there is a linear relationship between TEX₈₆ and BIT values in these sediments, suggesting an influence of terrigenous isoGDGTs on TEX₈₆. This approach has been used elsewhere to assess terrigenous input and can help determine whether to discard TEX₈₆ values (e.g., Douglas et al., 2014).

High BIT values may not always bias TEX₈₆. This is evident in ~56 Ma old sediments from Maryland, USA (covering the Paleocene-Eocene Thermal Maximum), where adjacent downcore sediment samples with high (>0.6) and low (<0.3) BIT values do not yield markedly different (<1.5°C) TEX₈₆-inferred temperature estimates (Inglis et al., 2023a). In this site, in situ marine production of brGDGTs may skew the BIT index toward higher values (see also Zhu et al., 2021), as is increasingly reported from modern marine environments (Ceccopieri et al., 2018; Dearing Crampton-Flood et al., 2019; Fietz et al., 2012; Herfort et al., 2006; Kaiser et al., 2015; Peterse et al., 2009; Schmidt et al., 2010; Sinninghe Damsté, 2016; Zhu et al., 2011). The production of brGDGTs in marine sediments and the water column can be identified (including for past environments) by higher relative abundances of brGDGTs with cyclopentane moieties and other indices (e.g., Liu et al., 2014; Sinninghe Damsté, 2016), which is potentially driven by the higher pH in marine sediments compared to most soils and peats. Elsewhere, high BIT index values can reflect a low production of crenarchaeol (Sparkes et al., 2015). In addition, brGDGTs can also be produced within riverine environments, and thus contribute to the brGDGT pool stored in coastal marine sediments (Dearing Crampton-Flood et al., 2021; French et al., 2015; Zell et al., 2013). Riverine brGDGTs are typically dominated by 6-methyl isomers compared to catchments soils (e.g., De Jonge et al., 2014), and their contribution to marine sediments can thus be identified by an increase in these compounds relative to the 5-methyl brGDGTs.

Taken together, this implies that the original threshold for excluding TEX₈₆ values (i.e., BIT >0.3 or 0.4) varies on a site-by-site basis and is not always the appropriate cut-off. In addition, a round-robin study showed large variation of BIT values reported by different laboratories for the same sediment extracts (up to 0.4 units on a scale of 0–1; Schouten et al., 2013a) due to different MS tuning (discussed in Bijl et al., 2025). As such, additional

approaches are needed to assess the impact of terrigenous isoGDGTs on TEX₈₆-based SSTs. For instance, the recent development of machine learning-based isoGDGT characterization tools has been used to characterize sources of isoGDGTs in deep-time marine sediments (e.g., the BIGMaC algorithm; Martínez-Sosa et al., 2023). Application of BIGMaC in sediments across the Paleocene-Eocene Thermal Maximum confirms that the threshold for identifying sediment samples with high terrigenous isoGDGT input could be much higher in some settings (BIT >0.6–0.7; Fokkema, Brinkhuis, et al., 2024; Inglis et al., 2023a), but this has not been investigated for other time intervals. Moving forward, we suggest using the wide range of indices outlined in Bijl et al. (2025) to assess the contribution and impacts of terrestrial-derived GDGTs in paleorecords.

8.6. Resuspension and Lateral Advection of isoGDGTs

Downslope transport via mass gravity flows (e.g., turbidites) can influence sedimentary TEX₈₆ values. These processes can mix material from different source regions and/or ages, potentially overprinting the primary TEX₈₆ temperature signal (Hartman et al., 2018; Littler et al., 2014). Marine sediments can also be prone to resuspension and lateral advection by bottom water currents, potentially affecting TEX₈₆-derived SST estimates (e.g., Xiao et al., 2023a). Planktonic foraminifera, due to their relatively large size and density, are less susceptible to lateral advection than isoGDGTs and other lipids. As such, the radiocarbon (¹⁴C) offset between isoGDGTs and planktonic foraminifera has been used to assess the impact of lateral advection on isoGDGT-based proxies. ¹⁴C ages of isoGDGTs are typically older than planktonic foraminifera from the same sample, but this offset varies spatially, with age offsets ranging from 820 ± 800 years (Bermuda Rise) to ~1280–1600 years (Santa Monica Basin; Shah et al., 2008). Mollenhauer et al. (2007, 2008) and Shah et al. (2008) found that the ¹⁴C-offset between crenarchaeol and planktonic foraminifera (950 ± 500 years) is much smaller than between alkenones and planktonic foraminifera (4,000 ± 2,000 years) in the same continental margin drift sediments, which was attributed to the lower preservation potential of isoGDGTs compared with alkenones. This suggests that isoGDGTs are less affected by lateral transport processes compared to alkenones. This is consistent with a multi-proxy biomarker (GDGTs, alkenones, *n*-alkanes) study from the Southern Ocean which suggested that isoGDGTs are less prone to lateral advection from the strong Antarctic Circumpolar Current than other biomarkers (Kim et al., 2009b). Visual particle tracking experiments have helped quantify potential isoGDGT transport biases for TEX₈₆ in the Mediterranean Sea and suggest that any bias arising from lateral advection at this location is small (<0.85°C) and within the calibration error of TEX₈₆ SST calibrations (Rice et al., 2022).

In summary, in regions with strong currents and drift sites (Xiao et al., 2023a), TEX₈₆ values may be affected by lateral transport, but overall the impact of lateral advection on TEX₈₆ appears to be minimal, especially compared to other temperature-sensitive biomarkers (e.g., alkenones). However, these conclusions are based on a relatively small number of studies, and thus further research is needed to constrain the effect of lateral transport on TEX₈₆ across a range of depositional regimes.

9. Diagenesis and Preservation Potential of Archaeal isoGDGTs

The oldest sediments reported to contain isoGDGTs are ~190 Ma old (Early Jurassic; Robinson et al., 2017), but preservation of isoGDGTs in (early) Mesozoic sediments remains sporadic. The fate of isoGDGTs is dependent on various dia- and catagenetic processes that begin during cell senescence and continue to take place until isoGDGT are completely degraded (as explained below; Figure 15a).

9.1. Loss of the Polar Head Group

The labile polar head group is prone to diagenesis, with observational and experimental evidence suggesting its loss on timescales from days to several millennia (Harvey et al., 1986; Lengger et al., 2012, 2014a; Liu et al., 2016; Xie et al., 2013). Polar head groups are bound via relatively weak linkages, that is, either a phosphatidic or a glycosidic bond, and are thus indicators of living or recently living microbial populations (Harvey et al., 1986; Logemann et al., 2011; Schouten et al., 2010; Xie et al., 2013). The effect of oxic versus anoxic conditions on the degradation of archaeal IPLs has been studied experimentally for archaeal diether lipids, showing that oxygen exposure increased the degradation rate compared to anoxic conditions (Harvey et al., 1986; Xie et al., 2013). For IPL-isoGDGTs, the effect of oxygen exposure has been tested using partially oxidized organic matter-rich turbidites (Lengger et al., 2013), showing that concentrations of IPL-isoGDGTs decreased by two to three orders of magnitude upon oxygen exposure. IsoGDGTs containing glycosidically bound polar head

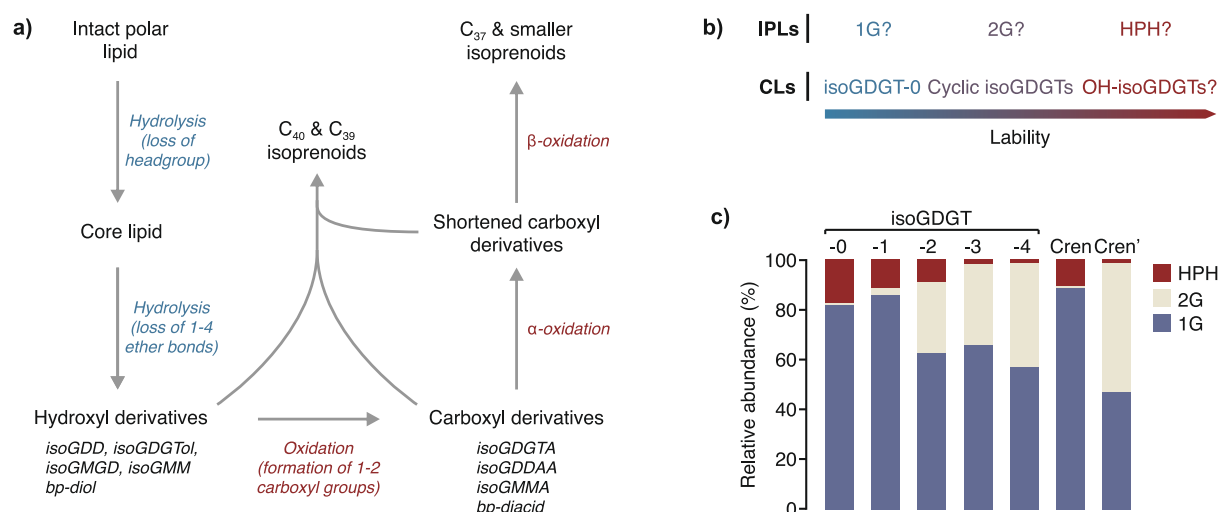


Figure 15. Diagenesis of isoGDGTs. (a) Conceptual model of isoGDGT degradation processes (blue: hydrolysis; red: β -oxidation) and products (adapted from Liu et al., 2016). Abbreviations: GDD, glycerol dibiphytanol diether; GDGTol, glycerol dialkyl glycerol triether alcohol; GMD, glycerol monobiphytanyl glycerol diether; GMM, glycerol monobiphytanol monoether; bp-diol, biphytanic diol; GDGTA, glycerol dialkyl glycerol triether acid; GDAA, glycerol dibiphytanol diether diacid; GMA, glycerol monobiphytanol monoether acid; bp-diacid, biphytanic diacid. (b) Conceptualization of isoGDGT lability, with hexose-phosphohexose (HPH) being the most labile and monoglycosyl (1G) being the least labile intact polar lipid (IPL) isoGDGTs, OH-isoGDGTs potentially being the most labile core isoGDGTs, and isoGDGTs containing rings being more labile than isoGDGT-0. Question marks denote that the relative lability of these compounds have not been tested experimentally. (c) Distribution of core isoGDGTs by IPL headgroup type in an early stationary phase culture of *Nitrosopumilus maritimus* (Elling et al., 2014), showing that some isoGDGTs are preferentially bound to specific headgroups (note that IPL quantification is semi-quantitative and may vary between laboratories). Differential degradation of IPLs could thus impact TEX₈₆ records.

groups are thought to be relatively stable compared to those with phosphatidic head groups and thus better preserved in marine sediments, although direct experimental evidence is still lacking (Figure 15b; Lengger et al., 2012). The distribution of core isoGDGTs by IPL headgroup type in cultures of *Nitrosopumilus maritimus* and other *Nitrososphaeria* differs (Figure 15c; Elling et al., 2014, 2015; Schouten et al., 2012; Varma et al., 2024a), suggesting that differential degradation of different IPL headgroup types may affect the distribution of core isoGDGTs and TEX₈₆ values. For example, it has been suggested that a faster degradation rate of phosphohexose compared to mono- and dihexose headgroups may result in a relatively higher abundance of isoGDGT-1 in the core isoGDGT fraction resulting in TEX₈₆^L estimates biased toward lower temperatures in the Baltic Sea water column (Wittenborn et al., 2023).

9.2. Breakdown of Core isoGDGTs

Core isoGDGTs are diagenetically much more stable than IPL-isoGDGTs (Lengger et al., 2013), but diagenetic and catagenetic processes will eventually lead to their breakdown. Post-depositional exposure of marine sediments to oxygen leads to a decrease of core isoGDGT concentrations by two orders of magnitude (Huguet et al., 2009). As this breakdown may be selective to specific isoGDGTs, substantial post-depositional exposure to oxygen may impact TEX₈₆ values (Huguet et al., 2009), but this has not been observed in all settings (Kim et al., 2009a; Lengger et al., 2013). As brGDGTs are better preserved than isoGDGTs, perhaps owing to selective (mineral) protection, oxic degradation can also lead to an increase of BIT values in marine sediments (Huguet et al., 2008, 2009; Lengger et al., 2013).

A wide variety of sedimentary components that are structurally related to isoGDGTs have been identified as diagenetic by-products and can represent >50% of the pool of isoGDGT-related products (Liu et al., 2016). Apart from biphytane diols (Hoefs et al., 1997; Schouten et al., 1998) and biphytanic diacids (Meunier-Christmann, 1988) with 0–3 rings, glycerol dialkanol diethers (isoGDDs; i.e., components in which the isoGDGTs lack one glycerol moiety; Knappy & Keely, 2012; Liu et al., 2012b) were identified as more complex degradation product. In marine settings, isoGDDs are one order of magnitude less abundant than isoGDGTs and likely have mixed diagenetic and biosynthetic origins (de Bar, Rampen, et al., 2019; Hingley et al., 2024; Knappy & Keely, 2012; Liu et al., 2012b, 2016; Meador et al., 2014). IsoGDDs with a monoglycosidic polar head group

attached to the remaining glycerol moiety have also been identified in sediments and cultures (Meador et al., 2014) and are presumably derived from preferential cleavage of the ether bond relative to the glycosidic bond of monoglycosidic isoGDGTs (Zhu et al., 2024).

IsoGDGT-based proxies are used to reconstruct paleotemperatures and ocean biogeochemistry from sediments as old as ~190 Ma (Early Jurassic), yet their degradation by the hydrolysis of their ether bonds commences on much shorter timescales. Ether bonds can only be hydrolyzed under strongly acidic conditions and elevated temperatures, yet their presumed hydrolysis products are found in surface sediments (e.g., biphytane diols; Hoefs et al., 1997) and cultures of *Nitrosopumilus maritimus*, albeit in small amounts (<2%; Liu et al., 2016). Although these components could represent biosynthetic products, their accumulation during the stationary phase suggests a partial enzymatic source during cell senescence rather than formation exclusively via diagenesis. This may imply that ether bonds are broken by uncharacterized enzymes involved in the microbial degradation of core isoGDGTs. Liu et al. (2016) presented a diagenetic scheme (Figure 15a) illustrating three key reactions suggested to play a main role in the process: (a) hydrolysis of ether bonds, (b) oxidation of terminal hydroxy groups, and (c) α - and β -oxidation resulting in shortening of the biphytane chains. In this way, most of the diagenetic products encountered could be explained. The timing and conditions at which these reactions occur remain elusive.

During catagenesis, isoGDGTs begin to undergo thermal cracking. Artificial maturation experiments using hydrous pyrolysis indicate that isoGDGTs are completely decomposed at 300°C after only 72 hr (Schouten et al., 2004). When C-C bonds start to break above 240°C, there is preferential degradation of isoGDGTs with cyclopentane moieties (Figure 15b; Schouten et al., 2004), leading to lower-than-expected TEX₈₆ values and reconstructed temperatures (up to 0.25 TEX₈₆ units; Schouten et al., 2004). This has been suggested as an explanation for anomalous TEX₈₆ values in Early Cretaceous sediments with elevated thermal maturity (Bottini et al., 2015). As such, Schouten et al. (2004) recommend using other biomarker proxies to constrain thermal maturity and hence the potential bias in TEX₈₆ values. They proposed excluding TEX₈₆ values in sediments with a relatively high abundance of 22S-hopanes (i.e., 22S/(22S + 22R) hopane ratios >0.2) or $\alpha\beta$ and $\beta\alpha$ hopanes (i.e., hopane $\beta\beta$ /($\beta\beta$ + $\alpha\beta$ + $\beta\alpha$) ratios <0.5; Schouten et al., 2004). How artificial maturation experiments, as conducted by Schouten et al. (2004), relate to natural maturation at geological timescales remains unclear, as sometimes adjacent sediment horizons with different thermal maturity ratios below and above the thresholds have similar TEX₈₆ values (Naafs & Pancost, 2016). In addition, hopane-based thermal maturity ratios may also be influenced by other processes; for example, transient changes in the input of petrogenic carbon (Hollingsworth et al., 2024; Inglis et al., 2023a). As such, we recommend using additional thermal maturity indices (such as vitrinite reflectance, RockEval Pyrolysis, and palynomorph indices) when applying TEX₈₆ to deep-time sediments. Despite these caveats, it is clear that the preservation of isoGDGTs in Cenozoic (66–0 Ma) and Mesozoic (252–66 Ma) sediments generally occurs in sediments with low thermal maturation (e.g., Mutterlose et al., 2010; Naafs & Pancost, 2016; Robinson et al., 2017).

Catagenesis results in the breakdown of isoGDGTs into their constitutive hydrocarbons. Head-to-head linked isoprenoid hydrocarbons—first identified in petroleum by Moldowan & Seifert (1979)—are thought to derive from archaeal membrane lipids, including isoGDGTs. Rowland (1990) showed that these hydrocarbons could be produced by laboratory maturation of biomass of methanogenic archaea. Pancost et al. (2008) demonstrated that isoGDGTs may become kerogen-bound and that artificial maturation using hydrous pyrolysis releases (a)cyclic biphytanes with a carbon isotopic signature indicative of MG-I *Nitrososphaeria*. Hence, when exposed to appropriate conditions, catagenetic reactions, including both ether and C-C bond cleavage, can produce isoprenoid hydrocarbons that can be linked back to archaea in the original depositional environment.

The degradation of other isoGDGT derivatives, such as OH-isoGDGTs, has not been studied. It is likely that the tertiary hydroxyl group of OH-isoGDGTs is relatively labile and may be lost during diagenesis via a reduction step (Figure 15b). Potentially, this reduction could initially lead to the formation of unsaturated isoGDGTs, followed by reduction into “regular,” saturated isoGDGTs. OH-isoGDGTs have been reported from sediments as old as 94 Ma (Connock et al., 2022) but isoGDGTs have been observed in sediments of up to Jurassic age (190 Ma). Although this age gap could result from underreporting of OH-isoGDGT occurrence, it could also result from higher diagenetic lability of OH-isoGDGTs. The relative abundance of cyclopentane moieties and the connected IPL headgroups differ between isoGDGTs and OH-isoGDGTs (e.g., Elling et al., 2014; Liu et al., 2012c; Varma et al., 2024a). Therefore, (differential) degradation of OH-isoGDGTs into unsaturated or

saturated isoGDGTs could potentially result in biases of TEX₈₆ and OH-isoGDGT-based proxies. Future studies should explore the impact of thermal maturation on other isoGDGTs, including OH-isoGDGTs.

10. Other Applications of Archaeal Lipids and Their Isotopes in the Marine Realm

10.1. Insights Into the Ecology and Evolution of Marine Archaea

Beyond ocean temperature reconstructions, archaeal isoGDGTs have provided numerous insights into the metabolism and ecology of archaea in modern and past marine environments. Changes in the concentration of isoGDGTs in sediments has been used to infer changes in productivity. For example, concentrations of crenarchaeol and phytoplankton biomarkers (e.g., chlorins) are positively correlated in marine and lacustrine sediments, suggesting that productivity of MG-I.1a *Nitrososphaeria* is dependent on primary productivity (Fietz et al., 2011; Rice et al., 2026). During anoxic intervals, organic carbon-normalized crenarchaeol concentrations and mass accumulation rates increase, suggesting expansion of *Nitrososphaeria* and thus increased nitrification in response to ocean stratification and primary productivity (e.g., Castañeda et al., 2010; Elling et al., 2021; van Kemenade et al., 2025; Kuypers et al., 2001).

Besides productivity, isoGDGTs have also been used to infer the timing of major archaeal evolutionary events. The emergence of WCA and WCB ecotypes (see Section 4.1 for details) has been inferred from molecular clock dating of *Nitrososphaeria* phylogenies to ~300 Ma, coinciding with enhanced deep ocean oxygenation (Yang et al., 2021). Building on the observation that modern WCA and WCB have different isoGDGT distributions, recent work indicates that the shallow water ecotype (WCA) dominated in past warm climates (Rattanasriampaipong et al., 2022). Although it remains debated (see Section 7.1), it has also been suggested that crenarchaeol biosynthesis emerged as an adaptation to lower temperatures as *Nitrososphaeria* transitioned from a thermophilic to mesophilic habitat (Sinninghe Damsté et al., 2002).

10.2. Tracers of Archaea in the Sedimentary Biosphere

Besides water column processes, isoGDGTs have also been used to explore the dynamics of benthic archaea, including the sedimentary deep biosphere (often defined as >1 m sediment depth; Teske & Sørensen, 2008). Marine sediments comprise one of the largest ecosystems by biomass and host a diverse archaeal community (Baker et al., 2020). However, the contribution of benthic archaea, particularly in the deep biosphere, to the sedimentary lipid pool has been controversial (Schouten et al., 2010; Xie et al., 2013). As discussed before (Section 9.1), IPLs with glycosidic headgroups are thought to be more recalcitrant and are the dominant IPLs in deeply-buried sediments. In support of this view, phosphatidic isoGDGTs (e.g., HPH-GDGTs) but not glycosidic isoGDGTs (1G, 2G) are found mostly in surface sediments and degrade quickly with sediment depth (Carr et al., 2018; Lengger et al., 2012, 2014a). Other phosphatidic isoGDGTs and archaeols are common in energy-rich benthic systems such as cold seeps or euxinic systems (e.g., Besseling et al., 2018; Kellermann et al., 2016; Schubotz et al., 2011; Yoshinaga et al., 2015).

Experimental, observational, and modeling studies have suggested that IPL-isoGDGTs detected in marine sediments (including the deep biosphere) are largely fossilized detrital compounds derived from water column-dwelling MG-I.1a *Nitrososphaeria* (Lengger et al., 2012, 2014a; Schouten et al., 2010; Xie et al., 2013). However, stable carbon isotope analyses provide evidence for benthic archaea contributing to the sedimentary IPL pool. For example, de novo production of 1G-, 2G- and 3G-isoGDGTs and core isoGDGTs in marine surface sediments and the deep biosphere was demonstrated using radiotracer techniques (Evans et al., 2019). Intriguingly, Evans et al. (2019) observed one to two orders of magnitude higher radiotracer incorporation into 2G- and 3G-archaeols, indicating that glycosidic archaeols may be more suitable markers for benthic archaea than glycosidic isoGDGTs. Similarly, Lengger et al. (2014b) found low turnover rates of IPL-GDGTs in surface sediments based on low/no incorporation of ¹³C label in short-term incubation experiments. Based on the natural abundance of ¹³C in IPLs and core lipids, Zhu et al. (2021, 2024) further suggested that benthic archaea contribute isoGDGT-0 but not crenarchaeol or isoGDGT-1 to isoGDGT-3 to the IPL and core isoGDGT pools. The sources of glycosidic IPLs can be further elucidated by analyzing the composition and δ¹³C values of glycosidic head groups (Lin et al., 2010; Yoshinaga et al., 2015). For example, the dominant types of hexoses of sedimentary glycosidic isoGDGTs (Lin et al., 2010; Yoshinaga et al., 2015) differ from those found in MG-I.1a *Nitrososphaeria* pure cultures (Könneke et al., 2012). Production of glycosidic isoGDGTs by benthic archaea may also involve the recycling of isoGDGT core structures, such as crenarchaeol (Takano et al., 2010). In summary, this suggests that glycosidic IPLs in

sediments may represent a mixture of fossil and in situ contributions. Benthic IPL production could be an explanation for the presence of diverse lipids with core structures or headgroups not found in MG-I.1a *Nitrososphaeria*, such as isoBDGTs and isoPDGTs (see also Section 2; Coffinet et al., 2020; Dong et al., 2025; Meador et al., 2015), 1G-nonitol tetraethers (Lipp & Hinrichs, 2009), as well as unsaturated isoGDGTs (Yoshinaga et al., 2015; Zhu et al., 2014a) and methylated isoGDGTs (Sollich et al., 2017; Zhu et al., 2014b).

GDGT ^{14}C -labeling tracer experiments have provided further insights into the metabolisms of the benthic archaea and reveal that archaeal communities in sulfate-bearing sediments are dominated by heterotrophs, which preferentially assimilated acetate over dissolved inorganic carbon into isoGDGTs and archaeols, whereas archaeal communities in the methane-bearing zone were dominated by autotrophs, specifically hydrogenotrophic methanogens (Evans et al., 2019). Further, Bathyarchaeota were shown to degrade lignin based on label incorporation into isoGDGTs (Yu et al., 2018). These studies highlight the future potential of isoGDGTs in tracing metabolisms of benthic archaea and their contribution to biogeochemical cycles and the sedimentary (deep) biosphere.

10.3. Archaeal Lipid Isotopes as Tracers of Hydrology and Diverse Biogeochemical Cycles

The analysis of stable carbon and hydrogen isotopic compositions of isoGDGTs (or isoGDGT-derived biphytanes) and other archaeal lipids is cost- and labor-intensive but can provide key insights into the sources of isoGDGTs in the marine realm, both in the modern ocean and the geological record. Early studies used the $\delta^{13}\text{C}$ value of isoGDGT-derived biphytanes to track the ancestral expansion of modern MG-I.1a *Nitrososphaeria* during transient warming events and revealed that during Oceanic Anoxic Event (OAE) 1b (~111 Ma) up to 80 wt. % of bulk organic carbon was derived from archaeal biomass (Kuypers et al., 2001, 2002). More recently, $\delta^{13}\text{C}$ analysis of crenarchaeol—in combination with other biomarkers—has revealed the mechanisms responsible for anoxic water formation during sapropel events in the Mediterranean Sea (Elling et al., 2021). The $\delta^{13}\text{C}$ value of isoGDGTs and isoGDGT-derived biphytanes have also been used to identify contributions by methanotrophic archaea to the modern and ancient sedimentary isoGDGT pool (e.g., Birgel et al., 2006, 2008; Keller et al., 2025b; Pancost et al., 2000; Zhang et al., 2011; Zhu et al., 2024).

The $\delta^{13}\text{C}$ values of isoGDGTs have also been used to trace changes in the global carbon cycle. This is based on the observation that all cultured MG-I.1a *Nitrososphaeria* are obligate chemolithoautotrophs using hydrogen bicarbonate (HCO_3^-), the main component of dissolved inorganic carbon (Millero, 1995). Thus, the $\delta^{13}\text{C}$ values of their isoGDGTs should trace the $\delta^{13}\text{C}$ values of dissolved inorganic carbon. This has been leveraged to quantify carbon isotopic excursions and refine carbon emission scenarios across the Paleocene-Eocene Thermal Maximum (Elling et al., 2019; Schoon et al., 2013) and during the Miocene (Sabino et al., 2022). The carbon isotopic fractionation in MG-I.1a *Nitrososphaeria* may depend on CO_2 availability (He et al., 2022; Hurley et al., 2019; Pearson et al., 2019) and has been proposed as a potential proxy for $p\text{CO}_2$ (Hurley et al., 2019; Pearson et al., 2019). However, this approach remains in its infancy and has yet to be applied to the geological record.

The fractionation of the stable hydrogen isotopes in isoGDGTs has been studied in cultures of two thermophilic archaea (Harris et al., 2025; Kaneko et al., 2011; Rhim et al., 2024) and one culture of marine mesophilic MG-I.1a *Nitrososphaeria* (Leavitt et al., 2023). These studies collectively suggest that $\delta^2\text{H}$ values of isoGDGTs primarily reflects the $\delta^2\text{H}$ values of the growth water, while the influence of environmental and physiological factors is smaller than in eukaryotes and bacteria (Harris et al., 2025; Leavitt et al., 2023; Rhim et al., 2024). Therefore, $\delta^2\text{H}$ values of isoGDGTs may potentially be used as a future proxy for $\delta^2\text{H}$ values of ocean water. Although the variability of $\delta^2\text{H}$ values of water is low across large parts of the ocean, $\delta^2\text{H}$ values of isoGDGTs may, similarly to alkenones (e.g., van der Meer et al., 2007), prove useful for reconstructing large changes in salinity and/or freshwater inflow from rivers or melting sea ice, such as in marginal seas like the Black and the Baltic Sea or the Arctic Ocean. However, the few available $\delta^2\text{H}$ values of isoGDGTs from marine sediments (Kaneko et al., 2011; Keller et al., 2025a; Lengger et al., 2021) are more negative than those observed in *Nitrososphaeria* cultures (Leavitt et al., 2023), which suggests that additional factors, for example, metabolism (Leavitt et al., 2023; Wijker et al., 2019), impact the sedimentary $\delta^2\text{H}$ values of isoGDGTs. Therefore, proxy applications of $\delta^2\text{H}$ of isoGDGTs still require verification through additional culture experiments, modern environmental water and sediment samples, as well as paleorecords.

11. Workshop Consensus on the Application of isoGDGT Paleothermometers

11.1. Marine Group I *Nitrososphaeria* Are the Primary Source of isoGDGTs in the Modern Ocean

The TEX₈₆ proxy relies on the assumption that sedimentary isoGDGTs are produced predominantly by planktonic MG-I *Nitrososphaeria*, but previously it has been argued that other archaea, most notably MG-II Pos-eidoniales, produce isoGDGTs, including crenarchaeol and its isomer. However, the absence of the required biosynthetic genes in these archaea imply that Marine Group I *Nitrososphaeria* are the primary source of isoGDGTs in modern marine water columns (see Section 4), as originally proposed during the inception of the TEX₈₆ proxy (Schouten et al., 2002). Still, isoGDGTs can have multiple, spatially and temporally varying sources. Within Marine Group I *Nitrososphaeria*, different ecotypes (e.g., shallow vs. deep-dwelling) may contribute differentially to the water column isoGDGT signal (see Sections 11.2 and 11.3). Furthermore, benthic archaea may contribute isoGDGTs to the sedimentary signal (see Section 11.6).

11.2. Temperature Exerts First-Order Control on isoGDGT Cyclization

Several studies have highlighted potential non-thermal controls on isoGDGT cyclization (see Sections 6 and 7). Therefore, existing TEX₈₆ surface sediment calibrations likely amalgamate a wide variety of other non-thermal factors (see Section 6), including changes in habitat depth, spatial variability in community composition, seasonality, substrate availability, and changes in export depth or efficiency, some of which were already highlighted in the first stage of TEX₈₆ proxy development (Schouten et al., 2002). However, despite these uncertainties, the empirical correlation between temperature and TEX₈₆ observed in modern surface sediments and mesocosms is supported by experiments testing the physiological response of MG-I.1a *Nitrososphaeria* in culture to different temperatures (Section 7), indicating that growth temperature exerts first-order control on the number of cyclopentane moieties in isoGDGTs in the modern realm.

11.3. IsoGDGTs Are Predominantly Exported From <250 m Water Depth

It is now increasingly common for TEX₈₆ values to be interpreted as subsurface signals (e.g., Lopes dos Santos et al., 2010; Rommerskirchen et al., 2011; van der Weijst et al., 2022). Consistent with this, isoGDGT production is typically highest near the base of the photic zone, at or just below the nitracline (generally ~50–250 m depth; Figures 8 and 9; cf. Rice et al., 2026). However, it is likely that isoGDGT export is more efficient at shallower depths due to incorporation of isoGDGTs into larger particles (marine snow, fecal pellets, or phytoplankton aggregates). Because maxima in both in situ isoGDGT production (~50–250 m) and primary production that can initiate isoGDGT export (~0–100 m) occur in the upper water column, the origin depth of most sedimentary isoGDGTs likely lies within the 0–250 m depth range at most sites. In relatively deep environments, as a conservative limit, isoGDGT production below 500 m contributes little to export flux, based on converging isoGDGT distributions in sediment traps below this depth. This is further supported by the lack of exceptionally high isoGDGT-2/isoGDGT-3 (>25) and isoGDGT-2/(isoGDGT-2+isoGDGT-3) ratios (>0.95) in most marine sediments (Figure 10). We therefore suggest that future studies that employ subsurface calibrations use those calibrated no deeper than 250 m depth. Crucially, as shallow subsurface temperature variability typically is strongly coupled to that of the sea surface, TEX₈₆ can still be interpreted as representing SST variability and trends, assuming that this relationship holds true in the paleorecords (as argued by Ford et al., 2015; Ho & Laepple, 2015).

When reconstructing absolute SSTs, an assumption must be made about whether TEX₈₆ is capturing SST or shallow subsurface temperature—this could potentially be guided using other temperature indicators such as the U^{K'}₃₇ SST proxy. However, this may be challenging in sediments where the upper temperature limit of U^{K'}₃₇ is close to saturation (Müller et al., 1998; Prah et al., 1988), and/or where alkenones are rare or absent (typically in sediments >50 Ma; Brassell, 2014). In these cases, comparing TEX₈₆-derived SSTs alongside inorganic geochemical SST estimates derived from calcite δ¹⁸O, Δ₄₇, and/or Mg/Ca measured on various species of planktonic foraminifera could also help assess whether TEX₈₆ is capturing SST or shallow subsurface temperature. This is because different species of planktonic foraminifera calcify at different water depths (e.g., mixed layer, thermocline, sub-thermocline), such that geochemical analysis of taxa living at different depth habitats can be used to reconstruct surface ocean temperature profiles (Hertzberg et al., 2016). As the reconstruction of ocean temperatures from multiple water depths (using δ¹⁸O and/or Mg/Ca of foraminifera) is increasingly commonplace (e.g., Frieling et al., 2017; Hertzberg et al., 2016; Inglis et al., 2023b), this could help to reconstruct changes in

isoGDGT export production depth. However, inorganic geochemical proxies also carry large uncertainties in deep time (e.g., Mg/Ca composition of seawater, calcite diagenesis etc; Hollis et al., 2019), suggesting this approach should be only undertaken when these biases can be constrained or excluded.

11.4. Culture Data May Guide the TEX₈₆-SST Response Beyond the Modern Range

Within the modern ocean calibration range (i.e., TEX₈₆ < 0.73), linear and non-linear isoGDGT-based temperature calibrations—most often BAYSPAR and TEX₈₆^H generally yield similar SST estimates (Kim et al., 2010; Tierney & Tingley, 2014) but diverge when TEX₈₆ values exceed the modern range (SST > 30°C, TEX₈₆ > 0.73). This has major implications for the application of TEX₈₆ in warmer-than-modern climates, especially the Eocene (~56–34 Ma) and Cretaceous (~143–66 Ma; e.g., Cramwinckel et al., 2018; Naafs & Pancost, 2016; O'Brien et al., 2017). Mesocosm and pure culture experiments demonstrate that isoGDGT-producing archaea can thrive at temperatures beyond those of the present-day ocean and that TEX₈₆ responds to increasing temperature in the range between 30 and 40°C (see Section 7). However, there are currently few data points available in this temperature range for both cultures and mesocosms. Further, in both mesocosms and pure cultures, the fractional abundance of the crenarchaeol isomer was much lower than expected based on the sedimentary TEX₈₆ and temperature correlation (Elling et al., 2015; Qin et al., 2015; Schouten et al., 2007b; Wuchter et al., 2004). Finally, mesocosm experiments have been performed only for two regions, while culture experiments cover only a small phylogenetic range, that is, not representative of many marine environments. As such, mesocosm and culture data have been rarely used as calibrations for paleoclimate reconstructions. Despite this, the TEX₈₆-temperature responses of mesocosms and cultures reflect *Nitrososphaeria* temperature adaptation and may help guide extrapolation beyond the calibrated temperature range.

11.5. Re-Evaluating Non-Thermal Overprints and Existing Thresholds

Archaeal-based isoGDGT proxies can be influenced by various non-thermal overprints. However, the criteria for excluding problematic data vary between studies and are not always well constrained. Terrigenous input of isoGDGTs can affect TEX₈₆ values and previous work suggested that marine sediments with BIT values > 0.4 should not be used for SST reconstructions. However, this threshold was specific to a single depositional system (the Congo Fan) and depends on the composition of isoGDGTs in the surrounding catchment (see Section 8), suggesting that better constraints on the threshold are needed. Thus, we recommend that all TEX₈₆ reconstructions are validated not only using BIT values, but by critically assessing the depositional environment alongside a comparison with other GDGT-based proxies (e.g., ΔRI, correlations of TEX₈₆ vs. BIT) and/or other tools (e.g., BIGMaC, compound-specific stable isotopic analysis) to help evaluate the possible terrigenous input biases in the record (see Section 8.5).

The impact of methanogenesis on sedimentary isoGDGT distributions likely varies by depositional and oceanographic setting. Previous studies used the %isoGDGT-0 (or isoGDGT-0/Cren ratios) as an indicator of methanogen overprint. Pure and enrichment cultures of *Nitrososphaeria* produce %isoGDGT-0 up to 67% (see Section 8.3), suggesting that higher values could indicate exogenous sources of isoGDGT-0. However, isoGDGT-0 also occurs in a diverse range of non-methanogenic archaea (see Section 2). Therefore, a high %isoGDGT-0 cannot be taken as direct evidence for methanogen contributions. Furthermore, many mesophilic methanogens do not biosynthesize cyclic isoGDGTs, suggesting limited impact on TEX₈₆. In contrast, the impact of anaerobic methanotrophy on sedimentary isoGDGT distributions is more likely to bias TEX₈₆ values, but its impact will vary substantially depending on the environment (e.g., anoxic basin, cold seep; see Section 8.2). We suggest that samples with MI values > 0.3 should be used with caution when estimating SST. Because isoGDGT distributions may already be impacted at MI values below 0.3, we advocate using other biomarkers and ideally their stable carbon isotopic composition (e.g., archaeol, isoGDGTs, or isoGDGT/derived biphytanes) to exclude a significant contribution from anaerobic methanotrophs.

Lateral advection appears to only have a small impact on TEX₈₆ values (< 0.85°C) and is only likely to be problematic in sites characterized by very high energy currents (e.g., drift sediments; see Section 8.6). Similarly, the impact of benthic production and/or recycling upon isoGDGT-based temperature proxies is also considered to be limited given that benthic isoGDGT lipids are more susceptible to degradation than fossil isoGDGTs. However, lateral advection and benthic production has been studied only at few sites and further research is needed to constrain their impact on TEX₈₆ across a broader range of depositional regimes.

11.6. Best Practices for Studies of isoGDGTs and TEX₈₆

More than two decades of research on TEX₈₆ and other isoGDGT-based paleotemperature proxies have led to the development of diverse tools for interpreting isoGDGT paleorecords. For example, various indices (e.g., BIT, ΔRI, MI) have been used to assess non-temperature effects on TEX₈₆. We recommend the consistent application of such tools to flag anomalous isoGDGT distributions (see also Bijl et al., 2025). Development of such tools relies on large databases of isoGDGT and brGDGT distributions as well as metadata. However, many published paleorecords report TEX₈₆ values but do not include isoGDGT fractional abundances, peak areas, or concentrations or are missing metadata (e.g., water depth), as do parts of the global surface sediment databases used for calibrations (Figure 6). Therefore, we recommend reporting all isoGDGT (and ideally brGDGT) data as well as metadata, ideally in a (community-)curated, centralized database. In deep-time marine sediments with elevated thermal maturity (mostly limited to Mesozoic sediments), thermal maturity ratios (e.g., hopane $\alpha\beta/(\alpha\beta + \beta\alpha + \beta\beta)$ and/or 22S/22S + 22R ratios; Schouten et al., 2004) should be reported to evaluate the potential impact of diagenesis and catagenesis on TEX₈₆ values. Finally, inclusion of a wider analytical window (i.e., using full scan mode or including non-TEX₈₆ lipids in single ion monitoring analyses) will help future-proof these analyses and provide the foundational data for the development of new tools and calibrations. Recommendations for sampling, processing, analyses, interpretation, and archiving have recently been published by Bijl et al. (2025).

12. Future Research Directions

12.1. Advances in the Analysis of isoGDGTs

Conventional isoGDGT analysis is based on the extraction of bulk sediment, typically grams of sediment or milligrams of suspended particulate matter. This limits spatial and temporal sampling resolution. Mass spectrometry imaging can overcome this by revealing the micrometer-scale distribution of lipids in a sediment sample (Alfken et al., 2019) and can resolve up to seasonal variability in laminated sedimentary sequences (Alfken et al., 2020; Napier et al., 2022). This can provide unique insights into past climate variability but also help better understand the mechanisms that govern isoGDGT distributions in marine environments (Alfken et al., 2020; Napier et al., 2022). In addition, mapping the microscale distribution of isoGDGTs in sinking particles may inform how these compounds are delivered to the ocean floor and incorporated into the sedimentary archive. However, this approach is unable to differentiate between crenarchaeol and its isomers, and thus currently uses an alternative temperature index (crenarchaeol-caldarchaeol tetraether index, CCaT) based upon the ratio of isoGDGT-0 and crenarchaeol, which can be further confounded by the diverse sources of GDGT-0 (see Sections 2 and 8). As mass spectrometry imaging of archaeal lipids has so far mostly been applied to laminated sediments, its broader applicability in non-laminated or bioturbated settings remains to be tested (Viola et al., 2025).

Apart from core isoGDGTs, a wide variety of archaeal lipids have been detected in marine environments but only a small selection is currently utilized to study environmental change in the marine realm. Recent advances in high resolution mass spectrometry have the potential to illuminate an expanded structural diversity of isoGDGTs in marine environments. Archaeal lipid analysis typically involves manual peak integration of selected compounds. Automated, “untargeted” methods have recently been developed to identify novel lipid biomarkers in the marine water column (e.g., Collins et al., 2016; Ding et al., 2021; Kharbush et al., 2016; Zheng et al., 2025). Archaeal lipids are not typically covered by the publicly available databases and thus generation of new databases represents a logical next step (Rempfert et al., 2023; Yao et al., 2023; Zheng et al., 2025; Zuffa et al., 2024).

An additional dimension of chemical diversity can be added to the analysis of isoGDGTs by exploring the spatial arrangements they represent, that is, their different structural and stereoisomers. This can be done by application of special chemical degradation techniques (Gräther & Arigoni, 1995; Liu et al., 2019; Schouten et al., 1998) but most information is provided by compound isolation and application of 2D NMR (Sinninghe Damsté et al., 2002) or total synthesis (Holzheimer et al., 2021). Although time-consuming, such studies could significantly advance the GDGT field. A different approach may involve integrating ion mobility separation into existing (U)HPLC-MS based protocols to separate isomers, but initial efforts have not been able to achieve this (Law et al., 2021). Improvements in mass spectrometry technologies, together with strategic efforts of the community to enable stringent criteria for untargeted lipid analysis, will also be key for advancing our understanding of archaeal lipid distributions in large environmental data sets and archaeal cultures.

The carbon and hydrogen stable isotopic compositions of isoGDGTs can provide insights into the source of isoGDGTs in the marine realm, and be used to reconstruct changes in the carbon cycle and potentially hydrological changes (see Section 10.3). This information can be obtained from the complete tetraether structure, from individual biphytanes, and internally via position-specific or moiety-specific signatures. Most studies have used labor-intensive protocols, including ether cleavage followed by hydrogenation to generate biphytanes amenable to conventional GC-IRMS analysis of $\delta^{13}\text{C}$ (e.g., Hoefs et al., 1997; Lin et al., 2013; Schoon et al., 2013; Schouten et al., 1998) and $\delta^2\text{H}$ values of bulk isoGDGTs (e.g., Kaneko et al., 2011; Kellermann et al., 2012). Therefore, applications of isoGDGTs to paleo-records remain rare and have been limited in temporal resolution. Recent advances have the potential to simplify stable isotope analyses of individual isoGDGTs without the need for chemical degradation, which allows generation of $\delta^{13}\text{C}$ or $\delta^2\text{H}$ records with higher resolution. For example, the $\delta^{13}\text{C}$ values of intact isoGDGTs can be obtained by Spooling Wire Microcombustion-isotope ratio mass spectrometry (Pearson et al., 2016), whilst the $\delta^2\text{H}$ values of intact isoGDGTs can be obtained via high-temperature gas chromatography coupled to pyrolysis/isotope ratio mass spectrometry (Lengger et al., 2021) or by HPLC purification of isoGDGTs followed by ether cleavage (Keller et al., 2025a). Finally, high resolution mass spectrometry techniques have recently been developed for the direct isotopic analysis of archaeal lipids and other compounds by HPLC-MS, although such techniques do not yet reach the analytical precision of conventional GC-C-IRMS (Groninga et al., 2025; Neubauer et al., 2023). The aforementioned improvements in the throughput and specificity of archaeal lipid isotopic analysis provide new avenues for their application in paleoenvironmental reconstruction.

12.2. Biosynthesis-Led Insights to Identify the Sources of Diverse Tetraether Lipids

The recent identification of enzymes responsible for the formation of isoGDGTs has enabled identification of the sources of isoGDGTs in the water column (Lloyd et al., 2022; Zeng et al., 2019, 2022; see Section 4). However, the biosynthesis of crenarchaeol and its isomer remains elusive. Understanding the biosynthesis of crenarchaeol isomer(s) is additionally important because its relative abundance is used in the TEX_{86} proxy. Such knowledge could also help refine the evolutionary origins of *Nitrososphaeria* via a combined approach using the sedimentary record of crenarchaeol, phylogenetics, and molecular clocks.

The biosynthetic pathways of polar headgroups in (marine) archaea and their role in membrane adaptation should also be constrained. As the effect of core lipid structures on membrane fluidity is modulated by polar headgroups (Chong, 2010) membrane adaptation mechanisms can only be fully understood and applied to understand environmental lipid distributions when the roles of polar headgroups are constrained. With few exceptions (e.g., Garcia et al., 2024), the enzymes responsible for other isoGDGT modifications such as side chain hydroxylation (relevant to OH-isoGDGTs) and (glycerol) methyltransferases (relevant to isoBDGTs and isoPDGTs) remain unknown. Identification of these enzymes will be required to define sources of these compounds, evaluate their proxy potential, and understand the various mechanisms archaea employ to modulate their cell membrane.

Recent advances in ultra-high resolution mass spectrometry also have the potential to reveal the internal isotopic patterning of geobiomolecules and could provide clues on biosynthetic pathways and source organisms. The use of Fourier transform mass spectrometers, particularly Orbitrap systems, provides sufficient mass resolution to distinguish between nearly isobaric interferences for compounds containing H, C, N, O, and/or S isotopes (Eiler et al., 2017). Combined with tandem mass spectrometry, intramolecular carbon isotopic signatures can therefore become accessible (Neubauer et al., 2023) and shed new lights on biosynthetic pathways.

12.3. Impact of isoGDGT Diagenesis and Catagenesis on isoGDGT Proxies

IsoGDGT-based proxies are used to reconstruct paleotemperatures and ocean biogeochemistry from ~190 Ma (Early Jurassic) to present. However, isoGDGT degradation products can also be found in recent sediments and even cultures, implying that isoGDGTs may be enzymatically degraded during early diagenesis (see Section 9). Experimental evidence to support this is lacking and it is unclear how the differential degradation of glyco-versus phospholipid isoGDGTs affects the distribution of core isoGDGTs in surface sediments. How early diagenetic degradation of core and IPL-isoGDGTs manifests itself in surface sediment calibrations and affects proxy reconstructions (e.g., TEX_{86} , MI) remains to be studied. OH-isoGDGTs are increasingly used for paleotemperature reconstruction, but these components contain a labile tertiary hydroxy group that seems prone to early diagenesis

through a dehydration reaction. Further studies are required to assess how diagenesis affects the distribution of OH-isoGDGTs, how this impacts isoGDGT-based proxies, and until what diagenetic stage these proxies can be applied with confidence.

Despite the widespread application of isoGDGT temperature proxies, the effect of (early) catagenesis on isoGDGTs remains largely unconstrained. For example, we still rely on a relatively simple hydrous pyrolysis experiment (Schouten et al., 2004) to assess what level of thermal maturity (measured by a hopane isomer ratio) we can apply isoGDGT proxies with confidence. We recommend that more effort should go into reaching a higher level of understanding of the effect of dia- and catagenesis on the distribution of sedimentary isoGDGTs. Laboratory incubation and simulation experiments should be conducted to investigate turnover, degradation patterns, and kinetic behaviors of isoGDGTs.

12.4. Toward a Holistic Understanding of isoGDGTs via Proxy System Models

Conventional paleoclimate reconstructions are based on statistical calibrations that link proxy measurements to climate parameters (i.e., an inverse modeling approach). However, other proxy communities are now reconsidering the mathematical and statistical approach toward proxy calibration by employing a forward modeling approach (e.g., Dee et al., 2015; Tierney & Tingley, 2014, 2018). However, this requires a mechanistic understanding of how temperature is imprinted into the sedimentary TEX₈₆ signal and will require answering several long-standing questions.

Firstly, the functional form of the TEX₈₆-SST relationship remains uncertain beyond the modern temperature range (>30°C; Section 5). We suggest that new and existing culture data (Figure 12; Section 7.1) could help guide the SST response beyond the modern range and determine the functional form of the TEX₈₆-SST relationship, especially above 30°C. The influence of spatial and temporal changes in water column structure, affecting both habitat and export depth, remain uncertain. The choice of calibration model can thus lead to fundamentally different interpretations of past climate dynamics, and therefore it is common to assume a plausible range of temperature estimates using multiple calibrations rather than selecting only one.

Secondly, in past warm climates, TEX₈₆ SST estimates can exceed 20°C in the high-latitudes regardless of the calibration used (e.g., Bijl et al., 2013; Jenkyns et al., 2012; O'Brien et al., 2017; Śliwińska et al., 2023; Sluijs et al., 2006, 2020), suggesting a potential seasonal bias. In the modern ocean, *Nitrososphaeria* growth follows a seasonal pattern (Section 6) whilst high-resolution orbitally-resolved TEX₈₆ SST records exhibit a seasonal bias in polar environments (Fokkema, Brinkhuis, et al., 2024; Fokkema, Agterhuis, et al., 2024). This potential bias could be further illuminated by developing similarly high-resolution empirical data sets and/or by culturing *Nitrososphaeria* under similar conditions (cf. Schouten et al., 2007b).

Thirdly, we must determine the physiological and ecological processes that operate in different oceanographic systems, across different timescales, and how these impact isoGDGT-based metrics. However, laboratory experiments linking community composition to isoGDGT distribution are largely based on a narrow range of diversity of *Nitrososphaeria*, representing only the coastal *Nitrosopumilus* clade (see Section 7.1). Therefore, cultured isolates representing a greater diversity of ecotypes of *Nitrososphaeria*, including shallow oligotrophic (WCA, see also Section 6.2), deep oligotrophic (WCB), polar, and restricted basin (e.g., Red Sea and/or the Mediterranean Sea), are required to understand how species- and ecotype-specific isoGDGT distributions contribute to isoGDGTs preserved in marine sediments, potentially using new metrics in addition to isoGDGT-2/(isoGDGT-2 + isoGDGT-3) ratios. At the community level, controlled mesocosm experiments paired with community characterization (cf. Schouten et al., 2007b) may help to distinguish the role of community composition versus environmental (ecophysiological) factors on the distribution of isoGDGTs—this could also help investigate the upper and lower limits of the TEX₈₆ proxy. Additionally, expanded spatial and latitudinal coverage of SPM and sediment trap studies are needed to constrain the ecological and oceanographic controls on the export depth and subsequent formation of the sedimentary TEX₈₆ signal. This knowledge is required before we can begin to quantify the effect of ecophysiological factors on TEX₈₆ values in the geological past.

Finally, a more comprehensive understanding of archaeal membrane lipid adaptation requires investigating a wider range of biomolecules, including OH-isoGDGTs. Additional priorities for future work include elucidating the physiological basis and confounding factors of novel isoGDGT-based proxies, including OH-isoGDGT-based ratios. For example, comparatively little is known about non-thermal effects on OH-isoGDGT proxies, including

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physiological factors (e.g., growth rate, nutrients) as well as their sources (WCA vs. WCB or other groups of archaea). Culturing and mesocosm experiments are needed to constrain how non-thermal factors affect OH-isoGDGTs, while combined genomic and intact polar lipid profiling of SPM and sediments can reveal the source of OH-isoGDGTs in the marine realm.

Ultimately, we strive toward an approach that embraces all (known) uncertainties and confounding factors in a proxy system model (Evans et al., 2013). The model would include priors for nutrient supply, the depth/season of export, dissolved oxygen, and water column structure. These priors can be informed by GDGT-based metrics that flag non-thermal effects (e.g., BIT, MI) as well as independent proxies for productivity and stratification that help constrain isoGDGT source and non-thermal overprints in the sedimentary record. Several studies have used the latter approach to assess confounding factors on isoGDGT paleothermometry (e.g., Huguet et al., 2006c; Wubben et al., 2024) and even qualitative constraints can be encoded as weak priors in an inverse framework. Finally, isoGDGT distributions can be assimilated with other (imperfect) temperature proxies with different sources of uncertainty in joint proxy inversion systems to reduce uncertainty (Bowen et al., 2020; The Cenozoic CO₂ Proxy Integration Project (CENCO2PIP) Consortium, 2023).

Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

Availability Statement

Data sets for this research are available at Zenodo (Elling et al., 2026).

References

- Adam, P. S., Borrel, G., Brochier-Armanet, C., & Gribaldo, S. (2017). The growing tree of Archaea: New perspectives on their diversity, evolution and ecology. *The ISME Journal*, 11(11), 2407–2425. <https://doi.org/10.1038/ismej.2017.122>
- Alfken, S., Wörmer, L., Lipp, J. S., Wendt, J., Schimmelmann, A., & Hinrichs, K.-U. (2020). Mechanistic insights into molecular proxies through comparison of subannually resolved sedimentary records with instrumental water column data in the Santa Barbara Basin, Southern California. *Paleoceanography and Paleoclimatology*, 35(10), e2020PA004076. <https://doi.org/10.1029/2020PA004076>
- Alfken, S., Wörmer, L., Lipp, J. S., Wendt, J., Taubner, H., Schimmelmann, A., & Hinrichs, K.-U. (2019). Micrometer scale imaging of sedimentary climate archives – Sample preparation for combined elemental and lipid biomarker analysis. *Organic Geochemistry*, 127, 81–91. <https://doi.org/10.1016/j.orggeochem.2018.11.002>
- Aloisi, G., Bouloubassi, I., Heijs, S. K., Pancost, R. D., Pierre, C., Sinninghe Damsté, J. S., et al. (2002). CH₄-consuming microorganisms and the formation of carbonate crusts at cold seeps. *Earth and Planetary Science Letters*, 203(1), 195–203. [https://doi.org/10.1016/S0012-821X\(02\)00878-6](https://doi.org/10.1016/S0012-821X(02)00878-6)
- Alves, R. J. E., Minh, B. Q., Urich, T., von Haeseler, A., & Schleper, C. (2018). Unifying the global phylogeny and environmental distribution of ammonia-oxidising archaea based on *amoA* genes. *Nature Communications*, 9(1), 1517. <https://doi.org/10.1038/s41467-018-03861-1>
- Auderset, A., Martínez-García, A., Tiedemann, R., Hasenfratz, A. P., Eglinton, T. I., Schiebel, R., et al. (2019). Gulf Stream intensification after the early Pliocene shoaling of the Central American Seaway. *Earth and Planetary Science Letters*, 520, 268–278. <https://doi.org/10.1016/j.epsl.2019.05.022>
- Auderset, A., Schmitt, M., & Martínez-García, A. (2020). Simultaneous extraction and chromatographic separation of n-alkanes and alkenones from glycerol dialkyl glycerol tetraethers via selective Accelerated Solvent Extraction. *Organic Geochemistry*, 143, 103979. <https://doi.org/10.1016/j.orggeochem.2020.103979>
- Aylward, F. O., & Santoro, A. E. (2020). Heterotrophic Thaumarchaea with small genomes are widespread in the dark ocean. *mSystems*, 5(3), e00415-20. <https://doi.org/10.1128/msystems.00415-20>
- Baker, B. J., Anda, V. D., Seitz, K. W., Dombrowski, N., Santoro, A. E., & Lloyd, K. G. (2020). Diversity, ecology and evolution of Archaea. *Nature Microbiology*, 5(7), 887–900. <https://doi.org/10.1038/s41564-020-0715-z>
- Bale, N. J., Palatinszky, M., Rijpstra, W. I. C., Herbold, C. W., Wagner, M., & Sinninghe Damsté, J. S. (2019). Membrane lipid composition of the moderately thermophilic ammonia-oxidizing archaeon “*Candidatus Nitrosotenuis uzonensis*” at different growth temperatures. *Applied and Environmental Microbiology*, 85(20), e01332-19. <https://doi.org/10.1128/AEM.01332-19>
- Bale, N. J., Sorokin, D. Y., Hopmans, E. C., Koenen, M., Rijpstra, W. I. C., Villanueva, L., et al. (2019). New insights into the polar lipid composition of extremely halo (alkali) philic euryarchaea from hypersaline lakes. *Frontiers in Microbiology*, 10, 377. <https://doi.org/10.3389/fmicb.2019.00377>
- Basse, A., Zhu, C., Versteegh, G. J. M., Fischer, G., Hinrichs, K.-U., & Mollenhauer, G. (2014). Distribution of intact and core tetraether lipids in water column profiles of suspended particulate matter off Cape Blanc, NW Africa. *Organic Geochemistry*, 72, 1–13. <https://doi.org/10.1016/j.orggeochem.2014.04.007>
- Bauersachs, T., & Schwark, L. (2016). Glycerol monoalkanedil diethers: A novel series of archaeal lipids detected in hydrothermal environments. *Rapid Communications in Mass Spectrometry*, 30(1), 54–60. <https://doi.org/10.1002/rcm.7417>
- Bauersachs, T., Weidenbach, K., Schmitz, R. A., & Schwark, L. (2015). Distribution of glycerol ether lipids in halophilic, methanogenic and hyperthermophilic archaea. *Organic Geochemistry*, 83–84, 101–108. <https://doi.org/10.1016/j.orggeochem.2015.03.009>
- Baumann, L. M. F., Taubner, R.-S., Bauersachs, T., Steiner, M., Schleper, C., Peckmann, J., et al. (2018). Intact polar lipid and core lipid inventory of the hydrothermal vent methanogens *Methanocaldococcus villosus* and *Methanothermococcus okinawensis*. *Organic Geochemistry*, 126, 33–42. <https://doi.org/10.1016/j.orggeochem.2018.10.006>

- Becker, K. W., Elling, F. J., Yoshinaga, M. Y., Söllinger, A., Urlich, T., & Hinrichs, K.-U. (2016). Unusual butane- and pentanetriol-based tetraether lipids in *Methanomassiliococcus luminyensis*, a representative of the seventh order of methanogens. *Applied and Environmental Microbiology*, 82(15), 4505–4516. <https://doi.org/10.1128/AEM.00772-16>
- Becker, K. W., Lipp, J. S., Zhu, C., Liu, X.-L., & Hinrichs, K.-U. (2013). An improved method for the analysis of archaeal and bacterial ether core lipids. *Organic Geochemistry*, 61, 34–44. <https://doi.org/10.1016/j.orggeochem.2013.05.007>
- Behrooz, L., Monteiro, F. M., Naafs, B. D. A., Taylor, K. W. R., Dickson, A. J., Graham, O. A., et al. (2024). North-East Peri-Tethyan water column deoxygenation and euxinia at the Paleocene Eocene Thermal Maximum. *Paleoceanography and Paleoclimatology*, 39(11), e2023PA004828. <https://doi.org/10.1029/2023PA004828>
- Belmar, L., Molina, V., & Ulloa, O. (2011). Abundance and phylogenetic identity of archaeoplankton in the permanent oxygen minimum zone of the eastern tropical South Pacific: Archaeal assemblages in an oxygen minimum zone. *FEMS Microbiology Ecology*, 78(2), 314–326. <https://doi.org/10.1111/j.1574-6941.2011.01159.x>
- Beman, J. M., Popp, B. N., & Alford, S. E. (2012). Quantification of ammonia oxidation rates and ammonia-oxidizing archaea and bacteria at high resolution in the Gulf of California and eastern tropical North Pacific Ocean. *Limnology and Oceanography*, 57(3), 711–726. <https://doi.org/10.4319/lo.2012.57.3.0711>
- Bentley, J. N., Ventura, G. T., Walters, C. C., Sievert, S. M., & Seewald, J. S. (2022). The influence of near-surface sediment hydrothermalism on the TEX₈₆ tetraether-lipid-based proxy and a new correction for ocean bottom lipid overprinting. *Biogeosciences*, 19(18), 4459–4477. <https://doi.org/10.5194/bg-19-4459-2022>
- Berg, C., Listmann, L., Vandieken, V., Vogts, A., & Jürgens, K. (2015). Chemoautotrophic growth of ammonia-oxidizing Thaumarchaeota enriched from a pelagic redox gradient in the Baltic Sea. *Frontiers in Microbiology*, 5. <https://doi.org/10.3389/fmicb.2014.00786>
- Berg, C., Vandieken, V., Thamdrup, B., & Jürgens, K. (2015). Significance of archaeal nitrification in hypoxic waters of the Baltic Sea. *The ISME Journal*, 9(6), 1319–1332. <https://doi.org/10.1038/ismej.2014.218>
- Bertagnolli, A. D., & Stewart, F. J. (2018). Microbial niches in marine oxygen minimum zones. *Nature Reviews Microbiology*, 16(12), 723–729. <https://doi.org/10.1038/s41579-018-0087-z>
- Besseling, M. A., Hopmans, E. C., Bale, N. J., Schouten, S., Sinninghe Damsté, J. S., & Villanueva, L. (2020). The absence of intact polar lipid-derived GDGTs in marine waters dominated by Marine Group II: Implications for lipid biosynthesis in Archaea. *Scientific Reports*, 10(1), 294. <https://doi.org/10.1038/s41598-019-57035-0>
- Besseling, M. A., Hopmans, E. C., Boschman, R. C., Sinninghe Damsté, J. S., & Villanueva, L. (2018). Benthic archaea as potential sources of tetraether membrane lipids in sediments across an oxygen minimum zone. *Biogeosciences*, 15(13), 4047–4064. <https://doi.org/10.5194/bg-15-4047-2018>
- Besseling, M. A., Hopmans, E. C., Koenen, M., van der Meer, M. T. J., Vreugdenhil, S., Schouten, S., et al. (2019). Depth-related differences in archaeal populations impact the isoprenoid tetraether lipid composition of the Mediterranean Sea water column. *Organic Geochemistry*, 135, 16–31. <https://doi.org/10.1016/j.orggeochem.2019.06.008>
- Biddle, J. F., Lipp, J. S., Lever, M. A., Lloyd, K. G., Sørensen, K. B., Anderso, R., et al. (2006). Heterotrophic Archaea Dominate Sedimentary Subsurface Ecosystems off Peru. *Proceedings of the National Academy of Sciences of the United States of America*, 103(10), 3846–3851. <https://doi.org/10.1073/pnas.0600035103>
- Bijl, P. K., Bendle, J. A. P., Bohaty, S. M., Pross, J., Schouten, S., Tauxe, L., et al. (2013). Eocene cooling linked to early flow across the Tasmanian Gateway. *Proceedings of the National Academy of Sciences of the United States of America*, 110(24), 9645–9650. <https://doi.org/10.1073/pnas.1220872110>
- Bijl, P. K., Śliwińska, K. K., Duncan, B., Huguet, A., Naeher, S., Rattanasriampaipong, R., et al. (2025). Reviews and syntheses: Best practices for the application of marine GDGTs as proxy for paleotemperatures: Sampling, processing, analyses, interpretation, and archiving protocols. *Biogeosciences*, 22(21), 6465–6508. <https://doi.org/10.5194/bg-22-6465-2025>
- Birgel, D., Elvert, M., Han, X., & Peckmann, J. (2008). ¹³C-depleted biphytanic diacids as tracers of past anaerobic oxidation of methane. *Organic Geochemistry*, 39(1), 152–156. <https://doi.org/10.1016/j.orggeochem.2007.08.013>
- Birgel, D., Peckmann, J., Klautzsch, S., Thiel, V., & Reitner, J. (2006). Anaerobic and Aerobic Oxidation of Methane at Late Cretaceous Seeps in the Western Interior Seaway, USA. *Geomicrobiology Journal*, 23(7), 565–577. <https://doi.org/10.1080/01490450600897369>
- Blaga, C. I., Reichart, G.-J., Heiri, O., & Sinninghe Damsté, J. S. (2009). Tetraether membrane lipid distributions in water-column particulate matter and sediments: A study of 47 European lakes along a north–south transect. *Journal of Paleolimnology*, 41(3), 523–540. <https://doi.org/10.1007/s10933-008-9242-2>
- Blumenberg, M., Seifert, R., Reitner, J., Pape, T., & Michaelis, W. (2004). Membrane lipid patterns typify distinct anaerobic methanotrophic consortia. *Proceedings of the National Academy of Sciences*, 101(30), 11111–11116. <https://doi.org/10.1073/pnas.0401188101>
- Boetius, A., Ravensschlag, K., Schubert, C. J., Rickert, D., Widdel, F., Gieseke, A., et al. (2000). A marine microbial consortium apparently mediating anaerobic oxidation of methane. *Nature*, 407(6804), 623–626. <https://doi.org/10.1038/35036572>
- Botini, C., Erba, E., Tiraboschi, D., Jenkyns, H. C., Schouten, S., & Sinninghe Damsté, J. S. (2015). Climate variability and ocean fertility during the Aptian Stage. *Climate of the Past*, 11(3), 383–402. <https://doi.org/10.5194/cp-11-383-2015>
- Bowen, G. J., Fischer-Femal, B., Reichart, G.-J., Sluijs, A., & Lear, C. H. (2020). Joint inversion of proxy system models to reconstruct paleo-environmental time series from heterogeneous data. *Climate of the Past*, 16(1), 65–78. <https://doi.org/10.5194/cp-16-65-2020>
- Brassell, S. C. (2014). Climatic influences on the Paleogene evolution of alkenones. *Paleoceanography*, 29(3), 255–272. <https://doi.org/10.1002/2013PA002576>
- Brochier-Armanet, C., Boussau, B., Gribaldo, S., & Forterre, P. (2008). Mesophilic crenarchaeota: Proposal for a third archaeal phylum, the Thaumarchaeota. *Nature Reviews Microbiology*, 6(3), 245–252. <https://doi.org/10.1038/nrmicro1852>
- Carr, S. A., Schubotz, F., Dunbar, R. B., Mills, C. T., Dias, R., Summons, R. E., & Mandernack, K. W. (2018). Acetoclastic Methanosaeta are dominant methanogens in organic-rich Antarctic marine sediments. *The ISME Journal*, 12(2), 330–342. <https://doi.org/10.1038/ismej.2017.150>
- Castañeda, I. S., Schefuß, E., Pätzold, J., Sinninghe Damsté, J. S., Weldeab, S., & Schouten, S. (2010). Millennial-scale sea surface temperature changes in the eastern Mediterranean (Nile River Delta region) over the last 27,000 years. *Paleoceanography*, 25(1), PA1208.
- Ceccopieri, M., Carreira, R. S., Wagener, A. L. R., Hefter, J. H., & Mollenhauer, G. (2018). On the application of alkenone- and GDGT-based temperature proxies in the south-eastern Brazilian continental margin. *Organic Geochemistry*, 126, 43–56. <https://doi.org/10.1016/j.orggeochem.2018.10.009>
- Chappe, B., Michaelis, W., Albrecht, P., & Ourisson, G. (1979). Fossil evidence for a novel series of archaeobacterial lipids. *Naturwissenschaften*, 66(10), 522–523. <https://doi.org/10.1007/BF00404868>
- Chaumeil, P.-A., Mussig, A. J., Hugenholtz, P., & Parks, D. H. (2022). GTDB-Tk v2: Memory friendly classification with the genome taxonomy database. *Bioinformatics*, 38(23), 5315–5316. <https://doi.org/10.1093/bioinformatics/btac672>

- Chen, A., & Poulter, C. D. (1993). Purification and characterization of farnesyl diphosphate/geranylgeranyl diphosphate synthase. A thermostable bifunctional enzyme from *Methanobacterium thermoautotrophicum*. *Journal of Biological Chemistry*, 268(15), 11002–11007. [https://doi.org/10.1016/S0021-9258\(18\)82085-3](https://doi.org/10.1016/S0021-9258(18)82085-3)
- Chen, J., Hu, P., Li, X., Yang, Y., Song, J., Li, X., et al. (2018). Impact of water depth on the distribution of iGDGTs in the surface sediments from the northern South China Sea: Applicability of TEX₈₆ in marginal seas. *Frontiers of Earth Science*, 12(1), 95–107. <https://doi.org/10.1007/s11707-016-0620-1>
- Chen, W., Mohtadi, M., Schefuß, E., & Mollenhauer, G. (2016). Concentrations and abundance ratios of long-chain alkenones and glycerol dialkyl glycerol tetraethers in sinking particles south of Java. *Deep Sea Research Part I: Oceanographic Research Papers*, 112, 14–24. <https://doi.org/10.1016/j.dsr.2016.02.010>
- Chen, Y., Yang, H., Zheng, F., Wu, R., Zhang, C., Naafs, B. D. A., et al. (2025). Temperature-dependent modulation of the methylation degree of (tetra)ester-linked membrane-spanning lipids in an *Acidobacterium*. *Geochimica et Cosmochimica Acta*, 401, 190–203. <https://doi.org/10.1016/j.gca.2025.05.019>
- Chen, Y., Zheng, F., Yang, H., Yang, W., Wu, R., Liu, X., et al. (2022). The production of diverse brGDGTs by an *Acidobacterium* providing a physiological basis for paleoclimate proxies. *Geochimica et Cosmochimica Acta*, 337, 155–165. <https://doi.org/10.1016/j.gca.2022.08.033>
- Chong, P. L.-G. (2010). Archaeobacterial bipolar tetraether lipids: Physico-chemical and membrane properties. *Chemistry and Physics of Lipids*, 163(3), 253–265. <https://doi.org/10.1016/j.chemphyslip.2009.12.006>
- Church, M. J., DeLong, E. F., Ducklow, H. W., Karner, M. B., Preston, C. M., & Karl, D. M. (2003). Abundance and distribution of planktonic *Archaea* and *Bacteria* in the waters west of the Antarctic Peninsula. *Limnology and Oceanography*, 48(5), 1893–1902. <https://doi.org/10.4319/l.2003.48.5.1893>
- Coffinet, S., Meador, T. B., Mühlena, L., Becker, K. W., Schröder, J., Zhu, Q.-Z., et al. (2020). Structural elucidation and environmental distributions of butanetriol and pentanetriol dialkyl glycerol tetraethers (BDGTs and PDGTs). *Biogeosciences*, 17(2), 317–330. <https://doi.org/10.5194/bg-17-317-2020>
- Collins, J. R., Edwards, B. R., Fredricks, H. F., & Van Mooy, B. A. S. (2016). LOBSTAHS: An Adduct-Based Lipidomics Strategy for Discovery and Identification of Oxidative Stress Biomarkers. *Analytical Chemistry*, 88(14), 7154–7162. <https://doi.org/10.1021/acs.analchem.6b01260>
- Comita, P. B., & Gagosian, R. B. (1983). Membrane lipid from deep-sea hydrothermal vent methanogen: A new macrocyclic glycerol diether. *Science*, 222(4630), 1329–1331. <https://doi.org/10.1126/science.222.4630.1329>
- Connock, G. T., Owens, J. D., & Liu, X.-L. (2022). Biotic induction and microbial ecological dynamics of Oceanic Anoxic Event 2. *Communications Earth & Environment*, 3(1), 136. <https://doi.org/10.1038/s43247-022-00466-x>
- Coolen, M. J. L., Abbas, B., van Bleijswijk, J., Hopmans, E. C., Kuypers, M. M. M., Wakeham, S. G., & Sinninghe Damsté, J. S. (2007). Putative ammonia-oxidizing Crenarchaeota in suboxic waters of the Black Sea: A basin-wide ecological study using 16S ribosomal and functional genes and membrane lipids. *Environmental Microbiology*, 9(4), 1001–1016. <https://doi.org/10.1111/j.1462-2920.2006.01227.x>
- Cramwinckel, M. J., Huber, M., Kocken, I. J., Agnini, C., Bijl, P. K., Bohaty, S. M., et al. (2018). Synchronous tropical and polar temperature evolution in the Eocene. *Nature*, 559(7714), 382–386. <https://doi.org/10.1038/s41586-018-0272-2>
- Crouch, E. M., Shepherd, C. L., Morgans, H. E. G., Naafs, B. D. A., Dallanave, E., Phillips, A., et al. (2020). Climatic and environmental changes across the early Eocene climatic optimum at mid-Waipara River, Canterbury Basin, New Zealand. *Earth-Science Reviews*, 200, 102961. <https://doi.org/10.1016/j.earscirev.2019.102961>
- Danovaro, R., Dell'Anno, A., Corinaldesi, C., Rastelli, E., Cavicchioli, R., Krupovic, M., et al. (2016). Virus-mediated archaeal hecatomb in the deep seafloor. *Science Advances*, 2(10), e1600492. <https://doi.org/10.1126/sciadv.1600492>
- Darfeuil, S., Ménot, G., Giraud, X., Rostek, F., Tachikawa, K., García, M., & Bard, É. (2016). Sea surface temperature reconstructions over the last 70 kyr off Portugal: Biomarker data and regional modeling. *Paleoceanography*, 31(1), 40–65. <https://doi.org/10.1002/2015PA002831>
- Davtian, N., Bard, E., Darfeuil, S., Ménot, G., & Rostek, F. (2021). The Novel hydroxylated tetraether index RI-OH' as a sea surface temperature proxy for the 160–45 ka BP period off the Iberian margin. *Paleoceanography and Paleoclimatology*, 36(3), e2020PA004077. <https://doi.org/10.1029/2020PA004077>
- Davtian, N., Ménot, G., Fagault, Y., & Bard, E. (2019). Western Mediterranean sea paleothermometry over the last glacial cycle based on the novel RI-OH index. *Paleoceanography and Paleoclimatology*, 34(4), 616–634. <https://doi.org/10.1029/2018pa003452>
- Dawson, K. S., Freeman, K. H., & Macalady, J. L. (2012). Molecular characterization of core lipids from halophilic archaea grown under different salinity conditions. *Organic Geochemistry*, 48, 1–8. <https://doi.org/10.1016/j.orggeochem.2012.04.003>
- Dearing Crampton-Flood, E., Peterse, F., & Sinninghe Damsté, J. S. (2019). Production of branched tetraethers in the marine realm: Svalbard fjord sediments revisited. *Organic Geochemistry*, 138, 103907. <https://doi.org/10.1016/j.orggeochem.2019.103907>
- Dearing Crampton-Flood, E., van der Weijst, C. M. H., van der Molen, G., Bouquet, M., Yedema, Y., Donders, T. H., et al. (2021). Identifying marine and freshwater overprints on soil-derived branched GDGT temperature signals in Pliocene Mississippi and Amazon River fan sediments. *Organic Geochemistry*, 154, 104200. <https://doi.org/10.1016/j.orggeochem.2021.104200>
- de Bar, M. W., de Nooijer, L. J., Schouten, S., Ziegler, M., Sluijs, A., & Reichert, G.-J. (2019). Comparing seawater temperature proxy records for the past 90 Myrs from the shallow shelf record Bass River, New Jersey. *Paleoceanography and Paleoclimatology*, 34(4), 455–475. <https://doi.org/10.1029/2018PA003453>
- de Bar, M. W., Rampen, S. W., Hopmans, E. C., Sinninghe Damsté, J. S., & Schouten, S. (2019). Constraining the applicability of organic paleotemperature proxies for the last 90 Myrs. *Organic Geochemistry*, 128, 122–136. <https://doi.org/10.1016/j.orggeochem.2018.12.005>
- Dee, S., Emile-Geay, J., Evans, M. N., Allam, A., Steig, E. J., & Thompson, D. M. (2015). PRYSM: An open-source framework for PRoxY system modeling, with applications to oxygen-isotope systems. *Journal of Advances in Modeling Earth Systems*, 7(3), 1220–1247. <https://doi.org/10.1002/2015MS000447>
- De Jonge, C., Stadnitskaia, A., Hopmans, E. C., Cherkashov, G., Fedotov, A., & Sinninghe Damsté, J. S. (2014). In situ produced branched glycerol dialkyl glycerol tetraethers in suspended particulate matter from the Yenisei River, Eastern Siberia. *Geochimica et Cosmochimica Acta*, 125, 476–491. <https://doi.org/10.1016/j.gca.2013.10.031>
- de la Torre, J. R., Walker, C. B., Ingalls, A. E., Könneke, M., & Stahl, D. A. (2008). Cultivation of a thermophilic ammonia oxidizing archaeon synthesizing crenarchaeol. *Environmental Microbiology*, 10(3), 810–818. <https://doi.org/10.1111/j.1462-2920.2007.01506.x>
- DeLong, E. F. (1992). Archaea in coastal marine environments. *Proceedings of the National Academy of Sciences of the United States of America*, 89(12), 5685–5689. <https://doi.org/10.1073/pnas.89.12.5685>
- DeLong, E. F., King, L. L., Massana, R., Murray, A., Schleper, C., & Wakeham, S. G. (1998). Dibiphytanyl ether lipids in nonthermophilic crenarchaeotes. *Applied and Environmental Microbiology*, 64(3), 1133–1138. <https://doi.org/10.1128/AEM.64.5.1986-1986.1998>
- De Rosa, M., De Rosa, S., & Gambacorta, A. (1977a). ¹³C-NMR assignments and biosynthetic data for the ether lipids of *Caldwellia*. *Phytochemistry*, 16(12), 1909–1912. [https://doi.org/10.1016/0031-9422\(77\)80094-0](https://doi.org/10.1016/0031-9422(77)80094-0)

- De Rosa, M., De Rosa, S., Gambacorta, A., Minale, L., & Bu'Lock, J. D. (1977). Chemical structure of the ether lipids of thermophilic acidophilic bacteria of the *Caldariella* group. *Phytochemistry*, 16(12), 1961–1965. [https://doi.org/10.1016/0031-9422\(77\)80105-2](https://doi.org/10.1016/0031-9422(77)80105-2)
- De Rosa, M., Esposito, E., Gambacorta, A., Nicolaus, B., & Bu'Lock, J. D. (1980). Effects of temperature on ether lipid composition of *Caldariella acidophila*. *Phytochemistry*, 19(5), 827–831. [https://doi.org/10.1016/0031-9422\(80\)85120-x](https://doi.org/10.1016/0031-9422(80)85120-x)
- De Rosa, M., & Gambacorta, A. (1988). The lipids of archaeobacteria. *Progress in Lipid Research*, 27(3), 153–175. [https://doi.org/10.1016/0163-7827\(88\)90011-2](https://doi.org/10.1016/0163-7827(88)90011-2)
- De Rosa, M., Gambacorta, A., Nicolaus, B., Chappe, B., & Albrecht, P. (1983). Isoprenoid ethers; backbone of complex lipids of the archaeobacterium *Sulfolobus solfataricus*. *Biochimica et Biophysica Acta (BBA) - Lipids and Lipid Metabolism*, 753(2), 249–256. [https://doi.org/10.1016/0005-2760\(83\)90014-0](https://doi.org/10.1016/0005-2760(83)90014-0)
- De Rosa, M., Gambacorta, A., Nicolaus, B., Ross, H. N. M., Grant, W. D., & Bu'Lock, J. D. (1982). An Asymmetric Archaeobacterial Diether Lipid from Alkaliphilic Halophiles. *Microbiology*, 128(2), 343–348. <https://doi.org/10.1099/00221287-128-2-343>
- De Rosa, M., Gambacorta, A., Nicolaus, B., Sodano, S., & Bu'Lock, J. D. (1980). Structural regularities in tetraether lipids of *Caldariella* and their biosynthetic and phyletic implications. *Phytochemistry*, 19(5), 833–836. [https://doi.org/10.1016/0031-9422\(80\)85121-1](https://doi.org/10.1016/0031-9422(80)85121-1)
- Ding, S., Bale, N. J., Hopmans, E. C., Villanueva, L., Arts, M. G. I., Schouten, S., & Sinninghe Damsté, J. S. (2021). Lipidomics of environmental microbial communities. II: Characterization using molecular networking and information theory. *Frontiers in Microbiology*, 12, 659315. <https://doi.org/10.3389/fmicb.2021.659315>
- Dong, L., Jing, Y., Hou, J., Zhou, J., Yu, T., Chen, S., et al. (2025). A dominant subgroup of marine Bathyarchaea assimilates organic and inorganic carbon into unconventional membrane lipids. *Nature Microbiology*, 10, 2579–2590. <https://doi.org/10.1038/s41564-025-02121-5>
- Douglas, P. M. J., Affek, H. P., Ivany, L. C., Houben, A. J. P., Sijp, W. P., Sluijs, A., et al. (2014). Pronounced zonal heterogeneity in Eocene southern high-latitude sea surface temperatures. *Proceedings of the National Academy of Sciences*, 111(18), 6582–6587. <https://doi.org/10.1073/pnas.1321441111>
- Dunkley Jones, T., Eley, Y. L., Thomson, W., Greene, S. E., Mandel, I., Edgar, K., & Bendle, J. A. (2020). OPTiMAL: A new machine learning approach for GDGT-based palaeothermometry. *Climate of the Past*, 16(6), 2599–2617. <https://doi.org/10.5194/cp-16-2599-2020>
- Eguchi, T., Nishimura, Y., & Kakinuma, K. (2003). Importance of the isopropylidene terminal of geranylgeranyl group for the formation of tetraether lipid in methanogenic archaea. *Tetrahedron Letters*, 44(16), 3275–3279. [https://doi.org/10.1016/s0040-4039\(03\)00627-0](https://doi.org/10.1016/s0040-4039(03)00627-0)
- Eiler, J., Cesar, J., Chimiak, L., Dallas, B., Grice, K., Griep-Raming, J., et al. (2017). Analysis of molecular isotopic structures at high precision and accuracy by Orbitrap mass spectrometry. *International Journal of Mass Spectrometry*, 422, 126–142. <https://doi.org/10.1016/j.ijms.2017.10.002>
- Ekiel, I., & Sprott, G. D. (1992). Identification of degradation artifacts formed upon treatment of hydroxydiether lipids from methanogens with methanolic HCl. *Canadian Journal of Microbiology*, 38(8), 764–768. <https://doi.org/10.1139/m92-124>
- Elling, F. J. (2015). *Factors controlling the lipid composition of marine planktonic Thaumarchaeota* (PhD Thesis). University of Bremen.
- Elling, F. J., Gottschalk, J., Doeana, K. D., Kusch, S., Hurley, S. J., & Pearson, A. (2019). Archaeal lipid biomarker constraints on the Paleocene–Eocene carbon isotope excursion. *Nature Communications*, 10(1), 4519. <https://doi.org/10.1038/s41467-019-12553-3>
- Elling, F. J., Hemingway, J. D., Kharbush, J. J., Becker, K. W., Polik, C. A., & Pearson, A. (2021). Linking diatom-diazotroph symbioses to nitrogen cycle perturbations and deep-water anoxia: Insights from Mediterranean sapropel events. *Earth and Planetary Science Letters*, 571, 117110. <https://doi.org/10.1016/j.epsl.2021.117110>
- Elling, F. J., Inglis, G., Davtian, N., Hurley, S., Naafs, B. D., O'Connor, L., et al. (2026). Archaeal tetraether lipids as tracers for past marine environmental change [Dataset]. *Paleoceanography and Paleoclimatology*. Zenodo. <https://doi.org/10.5281/zenodo.20702815>
- Elling, F. J., Könneke, M., Lipp, J. S., Becker, K. W., Gagen, E. J., & Hinrichs, K.-U. (2014). Effects of growth phase on the membrane lipid composition of the thaumarchaeon *Nitrosopumilus maritimus* and their implications for archaeal lipid distributions in the marine environment. *Geochimica et Cosmochimica Acta*, 141, 579–597. <https://doi.org/10.1016/j.gca.2014.07.005>
- Elling, F. J., Könneke, M., Mußmann, M., Greve, A., & Hinrichs, K.-U. (2015). Influence of temperature, pH, and salinity on membrane lipid composition and TEX86 of marine planktonic thaumarchaeal isolates. *Geochimica et Cosmochimica Acta*, 171, 238–255. <https://doi.org/10.1016/j.gca.2015.09.004>
- Elling, F. J., Könneke, M., Nicol, G. W., Stieglmeier, M., Bayer, B., Spieck, E., et al. (2017). Chemotaxonomic characterisation of the thaumarchaeal lipidome. *Environmental Microbiology*, 19(7), 2681–2700. <https://doi.org/10.1111/1462-2920.13759>
- Evans, M. N., Tolwinski-Ward, S. E., Thompson, D. M., & Anchukaitis, K. J. (2013). Applications of proxy system modeling in high resolution paleoclimatology. *Quaternary Science Reviews*, 76, 16–28. <https://doi.org/10.1016/j.quascirev.2013.05.024>
- Evans, T. W., Coffinet, S., Könneke, M., Lipp, J. S., Becker, K. W., Elvert, M., et al. (2019). Assessing the carbon assimilation and production of benthic archaeal lipid biomarkers using lipid-RIP. *Geochimica et Cosmochimica Acta*, 265, 431–442. <https://doi.org/10.1016/j.gca.2019.08.030>
- Fallet, U., Ullgren, J. E., Castañeda, I. S., van Aken, H. M., Schouten, S., Ridderinkhof, H., & Brummer, G.-J. A. (2011). Contrasting variability in foraminiferal and organic paleotemperature proxies in sedimenting particles of the Mozambique Channel (SW Indian Ocean). *Geochimica et Cosmochimica Acta*, 75(20), 5834–5848. <https://doi.org/10.1016/j.gca.2011.08.009>
- Ferrante, G., Ekiel, I., Patel, G. B., & Sprott, G. D. (1988). A novel core lipid isolated from the acetoclastic methanogen, *Methanoxanthus concilii* GP6. *Biochimica et Biophysica Acta (BBA) - Lipids and Lipid Metabolism*, 963(2), 173–182. [https://doi.org/10.1016/0005-2760\(88\)90278-0](https://doi.org/10.1016/0005-2760(88)90278-0)
- Fietz, S., Ho, S. L., & Hugué, C. (2020). Archaeal membrane lipid-based paleothermometry for applications in polar oceans. *Oceanography*, 33(2), 104–114. <https://doi.org/10.5670/oceanog.2020.207>
- Fietz, S., Ho, S. L., Hugué, C., Rosell-Melé, A., & Martínez-García, A. (2016). Appraising GDGT-based seawater temperature indices in the Southern Ocean. *Organic Geochemistry*, 102, 93–105. <https://doi.org/10.1016/j.orggeochem.2016.10.003>
- Fietz, S., Hugué, C., Bendle, J., Escala, M., Gallacher, C., Herfort, L., et al. (2012). Co-variation of crenarchaeol and branched GDGTs in globally-distributed marine and freshwater sedimentary archives. *Global and Planetary Change*, 92(93), 275–285. <https://doi.org/10.1016/j.gloplacha.2012.05.020>
- Fietz, S., Hugué, C., Rueda, G., Hambach, B., & Rosell-Melé, A. (2013). Hydroxylated isoprenoidal GDGTs in the Nordic Seas. *Marine Chemistry*, 152, 1–10. <https://doi.org/10.1016/j.marchem.2013.02.007>
- Fietz, S., Martínez-García, A., Rueda, G., Peck, V. L., Hugué, C., Escala, M., & Rosell-Melé, A. (2011). Crenarchaea and phytoplankton coupling in sedimentary archives: Common trigger or metabolic dependence? *Limnology and Oceanography*, 56(5), 1907–1916. <https://doi.org/10.4319/lo.2011.56.5.1907>
- Fokkema, C. D., Agterhuis, T., Gerritsma, D., de Goeij, M., Liu, X., de Regt, P., et al. (2024). Polar amplification of orbital-scale climate variability in the early Eocene greenhouse world. *Climate of the Past*, 20(6), 1303–1325. <https://doi.org/10.5194/cp-20-1303-2024>
- Fokkema, C. D., Brinkhuis, H., Peterse, F., & Sluijs, A. (2024). Orbital (hydro) climate variability in the ice-free early Eocene Arctic. *Paleoceanography and Paleoclimatology*, 39(12), e2024PA004907. <https://doi.org/10.1029/2024PA004907>

- Ford, H. L., Ravelo, A. C., Dekens, P. S., LaRiviere, J. P., & Wara, M. W. (2015). The evolution of the equatorial thermocline and the early Pliocene El Padre mean state. *Geophysical Research Letters*, 42(12), 4878–4887. <https://doi.org/10.1002/2015GL064215>
- Forster, A., Schouten, S., Moriya, K., Wilson, P. A., & Sinninghe Damsté, J. S. (2007). Tropical warming and intermittent cooling during the Cenomanian/Turonian oceanic anoxic event 2: Sea surface temperature records from the equatorial Atlantic. *Paleoceanography*, 22(1), PA1219. <https://doi.org/10.1029/2006PA001349>
- Francis, C. A., Roberts, K. J., Beman, J. M., Santoro, A. E., & Oakley, B. B. (2005). Ubiquity and diversity of ammonia-oxidizing archaea in water columns and sediments of the ocean. *Proceedings of the National Academy of Sciences*, 102(41), 14683–14688. <https://doi.org/10.1073/pnas.0506625102>
- French, D. W., Huguet, C., Turich, C., Wakeham, S. G., Carlson, L. T., & Ingalls, A. E. (2015). Spatial distributions of core and intact glycerol dialkyl glycerol tetraethers (GDGTs) in the Columbia River Basin and Willapa Bay, Washington: Insights into origin and implications for the BIT index. *Organic Geochemistry*, 88, 91–112. <https://doi.org/10.1016/j.orggeochem.2015.09.001>
- Frieling, J., Gebhardt, H., Huber, M., Adekeye, O. A., Akande, S. O., Reichart, G.-J., et al. (2017). Extreme warmth and heat-stressed plankton in the tropics during the Paleocene-Eocene Thermal Maximum. *Science Advances*, 3(3), e1600891. <https://doi.org/10.1126/sciadv.1600891>
- Fuhrman, J., & Davis, A. (1997). Widespread Archaea and novel Bacteria from the deep sea as shown by 16S rRNA gene sequences. *Marine Ecology Progress Series*, 150, 275–285. <https://doi.org/10.3354/meps150275>
- Fuhrman, J. A., McCallum, K., & Davis, A. A. (1992). Novel major archaeobacterial group from marine plankton. *Nature*, 356(6365), 148–149. <https://doi.org/10.1038/356148a0>
- Gabriel, J. L., & Chong, P. L. G. (2000). Molecular modeling of archaeobacterial bipolar tetraether lipid membranes. *Chemistry and Physics of Lipids*, 105(2), 193–200. [https://doi.org/10.1016/S0009-3084\(00\)00126-2](https://doi.org/10.1016/S0009-3084(00)00126-2)
- Galliker, P., Gräther, O., Rümmler, M., Fitz, W., & Arigoni, D. (1998). New structural and biosynthetic aspects of the unusual core lipids from archaeobacteria. In B. Kräutler, D. Arigoni, & B. T. Golding (Eds.), *Vitamin B12 and B12-proteins* (pp. 447–458). Wiley-VCH Verlag GmbH. <https://doi.org/10.1002/9783527612192.ch29>
- Gambacorta, A., Gliozzi, A., & De Rosa, M. (1995). Archaeal lipids and their biotechnological applications. *World Journal of Microbiology and Biotechnology*, 11(1), 115–131. <https://doi.org/10.1007/BF00339140>
- Garcia, A. A., Chadwick, G. L., Liu, X.-L., & Welander, P. V. (2024). Identification of two archaeal GDGT lipid-modifying proteins reveals diverse microbes capable of GMGT biosynthesis and modification. *Proceedings of the National Academy of Sciences*, 121(26), e2318761121. <https://doi.org/10.1073/pnas.2318761121>
- Gibson, R. A., van der Meer, M. T. J., Hopmans, E. C., Reysenbach, A.-L., Schouten, S., & Sinninghe Damsté, J. S. (2013). Comparison of intact polar lipid with microbial community composition of vent deposits of the Rainbow and Lucky Strike hydrothermal fields. *Geobiology*, 11(1), 72–85. <https://doi.org/10.1111/gbi.12017>
- Grant, G. R., Williams, J. H. T., Naeher, S., Seki, O., McClymont, E. L., Patterson, M. O., et al. (2023). Amplified surface warming in the south-west Pacific during the mid-Pliocene (3.3–3.0 Ma) and future implications. *Climate of the Past*, 19(7), 1359–1381. <https://doi.org/10.5194/cp-19-1359-2023>
- Gräther, O., & Arigoni, D. (1995). Detection of regioisomeric macrocyclic tetraethers in the lipids of *Methanobacterium thermoautotrophicum* and other archaeal organisms. *Journal of the Chemical Society, Chemical Communications*, (4), 405–406. <https://doi.org/10.1039/c39950000405>
- Groninga, J., Lipp, J., Song, M., & Hinrichs, K.-U. (2025). Isotopologue ratios identify ¹³C-depleted biomarkers in environmental samples impacted by Methane Turnover. *Rapid Communications in Mass Spectrometry*, 39(22), e10118. <https://doi.org/10.1002/rcm.10118>
- Guan, H., Liu, L., Birgel, D., Peckmann, J., Feng, D., & Li, S. (2024). Hydroxylated GDGTs-0 in marine methane seep environments: A putative indicator for archaeal methanogenesis. *Organic Geochemistry*, 198, 104862. <https://doi.org/10.1016/j.orggeochem.2024.104862>
- Guo, J., Wang, Z., Achterberg, E. P., Yuan, H., Song, J., Wang, Y., et al. (2024). Variations in isoprenoid tetraether lipids through the water column of the Western Pacific Ocean: Implications for sedimentary TEX₈₆ records. *Geochimica et Cosmochimica Acta*, 368, 24–33. <https://doi.org/10.1016/j.gca.2024.01.013>
- Hafenbradl, D., Keller, M., Thiericke, R., & Stetter, K. O. (1993). A novel unsaturated archaeal ether core lipid from the hyperthermophile *Methanopyrus kandleri*. *Systematic and Applied Microbiology*, 16(2), 165–169. [https://doi.org/10.1016/S0732-2020\(11\)80463-7](https://doi.org/10.1016/S0732-2020(11)80463-7)
- Hagemann, J. R., Lembke-Jene, L., Lamy, F., Vorrath, M.-E., Kaiser, J., Müller, J., et al. (2023). Upper-ocean temperature characteristics in the subantarctic southeastern Pacific based on biomarker reconstructions. *Climate of the Past*, 19(9), 1825–1845. <https://doi.org/10.5194/cp-19-1825-2023>
- Halamka, T. A., McFarlin, J. M., Younkin, A. D., Depoy, J., Dildar, N., & Kopf, S. H. (2021). Oxygen limitation can trigger the production of branched GDGTs in culture. *Geochimical Perspectives Letters*, 19, 36–39. <https://doi.org/10.7185/geochimlet.2132>
- Halamka, T. A., Raberg, J. H., McFarlin, J. M., Younkin, A. D., Mulligan, C., Liu, X.-L., & Kopf, S. H. (2023). Production of diverse brGDGTs by *Acidobacterium Solibacter usitatus* in response to temperature, pH, and O₂ provides a culturing perspective on brGDGT proxies and biosynthesis. *Geobiology*, 21(1), 102–118. <https://doi.org/10.1111/gbi.12525>
- Harning, D. J., Andrews, J. T., Belt, S. T., Cabedo-Sanz, P., Geirsdóttir, Á., Dildar, N., et al. (2019). Sea Ice Control on Winter Subsurface Temperatures of the North Iceland Shelf During the Little Ice Age: A TEX₈₆ Calibration Case Study. *Paleoceanography and Paleoclimatology*, 34(6), 1006–1021. <https://doi.org/10.1029/2018pa003523>
- Harning, D. J., Holman, B., Woelders, L., Jennings, A. E., & Sepúlveda, J. (2023). Biomarker characterization of the North Water Polynya, Baffin Bay: Implications for local sea ice and temperature proxies. *Biogeosciences*, 20(1), 229–249. <https://doi.org/10.5194/bg-20-229-2023>
- Harning, D. J., & Sepúlveda, J. (2024). Impact of non-thermal variables on hydroxylated GDGT distributions around Iceland. *Frontiers in Earth Science*, 12, 1430441. <https://doi.org/10.3389/feart.2024.1430441>
- Haro-Moreno, J. M., Rodríguez-Valera, F., López-García, P., Moreira, D., & Martín-Cuadrado, A.-B. (2017). New insights into marine group III Euryarchaeota, from dark to light. *The ISME Journal*, 11(5), 1102–1117. <https://doi.org/10.1038/ismej.2016.188>
- Harris, C. M., Kopf, S., Rhim, J. H., Cobban, A., Elling, F. J., Feng, X., et al. (2025). Lipid hydrogen isotope compositions primarily reflect growth water in the model archaeon *Sulfolobus acidocaldarius*. *Applied and Environmental Microbiology*, 91(4), e01983-24. <https://doi.org/10.1128/aem.01983-24>
- Hartman, J. D., Sangiorgi, F., Salabarnada, A., Peterse, F., Houben, A. J. P., Schouten, S., et al. (2018). Paleoceanography and ice sheet variability offshore Wilkes Land, Antarctica – Part 3: Insights from Oligocene–Miocene TEX₈₆-based sea surface temperature reconstructions. *Climate of the Past*, 14(9), 1275–1297. <https://doi.org/10.5194/cp-14-1275-2018>
- Harvey, H. R., Fallon, R. D., & Patton, J. S. (1986). The effect of organic matter and oxygen on the degradation of bacterial membrane lipids in marine sediments. *Geochimica et Cosmochimica Acta*, 50(5), 795–804. [https://doi.org/10.1016/0016-7037\(86\)90355-8](https://doi.org/10.1016/0016-7037(86)90355-8)
- He, J., Jia, J., Guo, W., & Jia, G. (2022). Archaeal tetraether lipids and their biphytane carbon isotope composition in sediments along an estuarine biogeochemical gradient. *Geochimica et Cosmochimica Acta*, 318, 452–467. <https://doi.org/10.1016/j.gca.2021.12.015>

- Heathcock, C. H., Finkelstein, B. L., Aoki, T., & Poulter, C. D. (1985). Stereostructure of the Archaeobacterial C₄₀ Diol. *Science*, 229(4716), 862–864. <https://doi.org/10.1126/science.3927485>
- Hemmi, H., Shibuya, K., Takahashi, Y., Nakayama, T., & Nishino, T. (2004). (S)-2,3-Di-O-geranylgeranylglyceryl Phosphate Synthase from the Thermoacidophilic Archaeon *Sulfolobus solfataricus*. *Journal of Biological Chemistry*, 279(48), 50197–50203. <https://doi.org/10.1074/jbc.m409207200>
- Herfort, L., Schouten, S., Abbas, B., Veldhuis, M. J. W., Coolen, M. J. L., Wuchter, C., et al. (2007). Variations in spatial and temporal distribution of Archaea in the North Sea in relation to environmental variables: Marine Archaea in the North Sea. *FEMS Microbiology Ecology*, 62(3), 242–257. <https://doi.org/10.1111/j.1574-6941.2007.00397.x>
- Herfort, L., Schouten, S., Boon, J. P., & Sinninghe Damsté, J. S. (2006). Application of the TEX₈₆ temperature proxy to the southern North Sea. *Organic Geochemistry*, 37(12), 1715–1726. <https://doi.org/10.1016/j.orggeochem.2006.07.021>
- Hernández-Sánchez, M. T., Woodward, E. M. S., Taylor, K. W. R., Henderson, G. M., & Pancost, R. D. (2014). Variations in GDGT distributions through the water column in the South East Atlantic Ocean. *Geochimica et Cosmochimica Acta*, 132, 337–348. <https://doi.org/10.1016/j.gca.2014.02.009>
- Hertzberg, J. E., Schmidt, M. W., Bianchi, T. S., Smith, R. W., Shields, M. R., & Marcantonio, F. (2016). Comparison of eastern tropical Pacific TEX₈₆ and *Globigerinoides ruber* Mg/Ca derived sea surface temperatures: Insights from the Holocene and Last Glacial Maximum. *Earth and Planetary Science Letters*, 434, 320–332. <https://doi.org/10.1016/j.epsl.2015.11.050>
- Hingley, J. S., Martins, C. C., Walker-Trivett, C., Adams, J. K., Naeher, S., Häggi, C., et al. (2024). The global distribution of Isoprenoidal Glycerol Dialkyl Diethers (isoGDDs) is consistent with a predominant degradation origin. *Organic Geochemistry*, 192, 104782. <https://doi.org/10.1016/j.orggeochem.2024.104782>
- Hinrichs, K.-U., Hayes, J. M., Sylva, S. P., Brewer, P. G., & DeLong, E. F. (1999). Methane-consuming archaeobacteria in marine sediments. *Nature*, 398(6730), 802–805. <https://doi.org/10.1038/19751>
- Hinrichs, K.-U., Pancost, R. D., Summons, R. E., Sprott, G. D., Sylva, S. P., Sinninghe Damsté, J. S., & Hayes, J. M. (2000). Mass spectra of sn-2-hydroxyarchaeol, a polar lipid biomarker for anaerobic methanotrophy. *Geochemistry, Geophysics, Geosystems*, 1(5), 2000GC000042. <https://doi.org/10.1029/2000gc000042>
- Ho, S. L., & Laepple, T. (2015). Glacial cooling as inferred from marine temperature proxies TEX₈₆^H and U^{K'}₃₇. *Earth and Planetary Science Letters*, 409, 15–22. <https://doi.org/10.1016/j.epsl.2014.10.033>
- Ho, S. L., & Laepple, T. (2016). Flat meridional temperature gradient in the early Eocene in the subsurface rather than surface ocean. *Nature Geoscience*, 9(8), 606–610. <https://doi.org/10.1038/ngeo2763>
- Ho, S.-L., & Laepple, T. (2017). Reply to “Eocene temperature gradients”. *Nature Geoscience*, 10(8), 539–540.
- Ho, S. L., Lin, Y.-S., Wang, P.-L., Chen, T.-T., Lee, P.-T., Wang, H.-H., et al. (2025). Methane Index and TEX₈₆ values in cold seep sediments: Implications for paleo-environmental reconstructions. *Geochimica et Cosmochimica Acta*, 391, 262–276. <https://doi.org/10.1016/j.gca.2024.12.033>
- Ho, S. L., Mollenhauer, G., Fietz, S., Martínez-García, A., Lamy, F., Rueda, G., et al. (2014). Appraisal of TEX₈₆ and TEX₈₆^L thermometries in subpolar and polar regions. *Geochimica et Cosmochimica Acta*, 131, 213–226. <https://doi.org/10.1016/j.gca.2014.01.001>
- Hoefs, M. J. L., Schouten, S., Leeuw, J. W. D., King, L. L., Wakeham, S. G., & Sinninghe Damsté, J. S. (1997). Ether lipids of planktonic archaea in the marine water column. *Applied and Environmental Microbiology*, 63(8), 3090–3095. <https://doi.org/10.1128/aem.63.8.3090-3095.1997>
- Hollibaugh, J. T., Gifford, S., Sharma, S., Bano, N., & Moran, M. A. (2011). Metatranscriptomic analysis of ammonia-oxidizing organisms in an estuarine bacterioplankton assemblage. *The ISME Journal*, 5(5), 866–878. <https://doi.org/10.1038/ismej.2010.172>
- Hollibaugh, J. T., Gifford, S. M., Moran, M. A., Ross, M. J., Sharma, S., & Tolar, B. B. (2014). Seasonal variation in the metatranscriptomes of a Thaumarchaeota population from SE USA coastal waters. *The ISME Journal*, 8(3), 685–698. <https://doi.org/10.1038/ismej.2013.171>
- Hollingsworth, E. H., Elling, F. J., Badger, M. P. S., Pancost, R. D., Dickson, A. J., Rees-Owen, R. L., et al. (2024). Spatial and temporal patterns in petrogenic organic carbon mobilization during the paleocene-eocene thermal maximum. *Paleoceanography and Paleoclimatology*, 39(2), e2023PA004773. <https://doi.org/10.1029/2023PA004773>
- Hollis, C. J., Dunkley Jones, T., Anagnostou, E., Bijl, P. K., Cramwinckel, M. J., Cui, Y., et al. (2019). The DeepMIP contribution to PMIP4: Methodologies for selection, compilation and analysis of latest Paleocene and early Eocene climate proxy data, incorporating version 0.1 of the DeepMIP database. *Geoscientific Model Development*, 12(7), 3149–3206. <https://doi.org/10.5194/gmd-12-3149-2019>
- Holzheimer, M., Sinninghe Damsté, J. S., Schouten, S., Havenith, R. W. A., Cunha, A. V., & Minnaard, A. J. (2021). Total synthesis of the alleged structure of crenarchaeol enables structure revision. *Angewandte Chemie*, 133(32), 17645–17654. <https://doi.org/10.1002/ange.202105384>
- Hopmans, E. C., Schouten, S., Pancost, R. D., van der Meer, M. T. J., & Sinninghe Damsté, J. S. (2000). Analysis of intact tetraether lipids in archaeal cell material and sediments by high performance liquid chromatography/atmospheric pressure chemical ionization mass spectrometry. *Rapid Communications in Mass Spectrometry*, 14(7), 585–589. [https://doi.org/10.1002/\(sici\)1097-0231\(20000415\)14:7<585::aid-rcm913>3.0.co;2-n](https://doi.org/10.1002/(sici)1097-0231(20000415)14:7<585::aid-rcm913>3.0.co;2-n)
- Hopmans, E. C., Schouten, S., & Sinninghe Damsté, J. S. (2016). The effect of improved chromatography on GDGT-based palaeoproxies. *Organic Geochemistry*, 93, 1–6. <https://doi.org/10.1016/j.orggeochem.2015.12.006>
- Hopmans, E. C., Weijers, J. W. H., Schefuß, E., Herfort, L., Sinninghe Damsté, J. S., & Schouten, S. (2004). A novel proxy for terrestrial organic matter in sediments based on branched and isoprenoid tetraether lipids. *Earth and Planetary Science Letters*, 224(1–2), 107–116. <https://doi.org/10.1016/j.epsl.2004.05.012>
- Hou, J., Wang, Y., Zhu, P., Yang, N., Liang, L., Yu, T., et al. (2023). Taxonomic and carbon metabolic diversification of Bathyarchaea during its coevolution history with early Earth surface environment. *Science Advances*, 9(27), eadf5069. <https://doi.org/10.1126/sciadv.adf5069>
- Hu, J., Meyers, P. A., Chen, G., Peng, P., & Yang, Q. (2012). Archaeal and bacterial glycerol dialkyl glycerol tetraethers in sediments from the Eastern Lau Spreading Center, South Pacific Ocean. *Organic Geochemistry*, 43, 162–167. <https://doi.org/10.1016/j.orggeochem.2011.10.012>
- Hugoni, M., Agogue, H., Taib, N., Domaizon, I., Moné, A., Galand, P. E., et al. (2015). Temporal dynamics of active prokaryotic nitrifiers and archaeal communities from river to sea. *Microbial Ecology*, 70(2), 473–483. <https://doi.org/10.1007/s00248-015-0601-z>
- Huguet, C., Cartes, J. E., Sinninghe Damsté, J. S., & Schouten, S. (2006). Marine crenarchaeal membrane lipids in decapods: Implications for the TEX₈₆ paleothermometer. *Geochemistry, Geophysics, Geosystems*, 7(11), Q11010. <https://doi.org/10.1029/2006gc001305>
- Huguet, C., de Lange, G. J., Gustafsson, Ö., Middelburg, J. J., Sinninghe Damsté, J. S., & Schouten, S. (2008). Selective preservation of soil organic matter in oxidized marine sediments (Madeira Abyssal Plain). *Geochimica et Cosmochimica Acta*, 72(24), 6061–6068. <https://doi.org/10.1016/j.gca.2008.09.021>
- Huguet, C., Fietz, S., & Rosell-Melé, A. (2013). Global distribution patterns of hydroxy glycerol dialkyl glycerol tetraethers. *Organic Geochemistry*, 57, 107–118. <https://doi.org/10.1016/j.orggeochem.2013.01.010>

- Huguet, C., Fietz, S., Rosell-Melé, A., Daura, X., & Costenaro, L. (2017). Molecular dynamics simulation study of the effect of glycerol dialkyl glycerol tetraether hydroxylation on membrane thermostability. *Biochimica et Biophysica Acta (BBA) - Biomembranes*, 1859(5), 966–974. <https://doi.org/10.1016/j.bbame.2017.02.009>
- Huguet, C., Hopmans, E. C., Febo-Ayala, W., Thompson, D. H., Sinninghe Damsté, J. S., & Schouten, S. (2006a). An improved method to determine the absolute abundance of glycerol dibiphytanyl glycerol tetraether lipids. *Organic Geochemistry*, 37(9), 1036–1041. <https://doi.org/10.1016/j.orggeochem.2006.05.008>
- Huguet, C., Kim, J.-H., de Lange, G. J., Sinninghe Damsté, J. S., & Schouten, S. (2009). Effects of long term oxic degradation on the $U^{K'}$, TEX_{86} and BIT organic proxies. *Organic Geochemistry*, 40(12), 1188–1194. <https://doi.org/10.1016/j.orggeochem.2009.09.003>
- Huguet, C., Kim, J.-H., Sinninghe Damsté, J. S., & Schouten, S. (2006c). Reconstruction of sea surface temperature variations in the Arabian Sea over the last 23 kyr using organic proxies (TEX_{86} and $U^{K'}$). *Paleoceanography*, 21(3), PA3003. <https://doi.org/10.1029/2005PA001215>
- Huguet, C., Martens-Habben, W., Urakawa, H., Stahl, D. A., & Ingalls, A. E. (2010). Comparison of extraction methods for quantitative analysis of core and intact polar glycerol dialkyl glycerol tetraethers (GDGTs) in environmental samples: Extraction methods for quantitative analysis of GDGTs. *Limnology and Oceanography: Methods*, 8(4), 127–145. <https://doi.org/10.4319/lom.2010.8.127>
- Huguet, C., Martrat, B., Grimalt, J. O., Sinninghe Damsté, J. S., & Schouten, S. (2011). Coherent millennial-scale patterns in $U^{K'}$ and TEX_{86} temperature records during the penultimate interglacial-to-glacial cycle in the western Mediterranean. *Paleoceanography*, 26(2), PA2218.
- Huguet, C., Schimmelmann, A., Thunell, R., Lourens, L. J., Sinninghe Damsté, J. S., & Schouten, S. (2007). A study of the TEX_{86} paleothermometer in the water column and sediments of the Santa Barbara Basin, California. *Paleoceanography*, 22(3), PA3203. <https://doi.org/10.1029/2006pa001310>
- Hurley, S. J., Close, H. G., Elling, F. J., Jasper, C. E., Gospodinova, K., McNichol, A. P., & Pearson, A. (2019). CO_2 -dependent carbon isotope fractionation in Archaea, Part II: The marine water column. *Geochimica et Cosmochimica Acta*, 261, 383–395. <https://doi.org/10.1016/j.gca.2019.06.043>
- Hurley, S. J., Elling, F. J., Könneke, M., Buchwald, C., Wankel, S. D., Santoro, A. E., et al. (2016). Influence of ammonia oxidation rate on thaumarchaeal lipid composition and the TEX_{86} temperature proxy. *Proceedings of the National Academy of Sciences*, 113(28), 7762–7767. <https://doi.org/10.1073/pnas.1518534113>
- Hurley, S. J., Lipp, J. S., Close, H. G., Hinrichs, K.-U., & Pearson, A. (2018). Distribution and export of isoprenoid tetraether lipids in suspended particulate matter from the water column of the Western Atlantic Ocean. *Organic Geochemistry*, 116, 90–102. <https://doi.org/10.1016/j.orggeochem.2017.11.010>
- Ingalls, A. E., Huguet, C., & Truxal, L. T. (2012). Distribution of Intact and Core Membrane Lipids of Archaeal Glycerol Dialkyl Glycerol Tetraethers among Size-Fractionated Particulate Organic Matter in Hood Canal, Puget Sound. *Applied and Environmental Microbiology*, 78(5), 1480–1490. <https://doi.org/10.1128/aem.07016-11>
- Inglis, G. N., Bhatia, R., Evans, D., Zhu, J., Müller, W., Matthey, D., et al. (2023b). Surface ocean cooling in the Eocene North Atlantic coincides with declining atmospheric CO_2 . *Geophysical Research Letters*, 50(24), e2023GL105448. <https://doi.org/10.1029/2023GL105448>
- Inglis, G. N., Collinson, M. E., Riegel, W., Wilde, V., Robson, B. E., Lenz, O. K., & Pancost, R. D. (2015b). Ecological and biogeochemical change in an early Paleogene peat-forming environment: Linking biomarkers and palynology. *Palaeogeography, Palaeoclimatology, Palaeoecology*, 438, 245–255. <https://doi.org/10.1016/j.palaeo.2015.08.001>
- Inglis, G. N., Farnsworth, A., Lunt, D., Foster, G. L., Hollis, C. J., Pagani, M., et al. (2015a). Descent toward the Icehouse: Eocene sea surface cooling inferred from GDGT distributions. *Paleoceanography*, 30(7), 1000–1020. <https://doi.org/10.1002/2014PA002723>
- Inglis, G. N., Martínez-Sosa, P., Tierney, J. E., Witkowski, C. R., Lyons, S., Baczynski, A. A., & Freeman, K. H. (2023a). Impact of organic carbon reworking upon GDGT temperature proxies during the Paleocene-Eocene Thermal Maximum. *Organic Geochemistry*, 183, 104644. <https://doi.org/10.1016/j.orggeochem.2023.104644>
- Inglis, G. N., & Tierney, J. E. (2020). *The TEX_{86} Paleotemperature Proxy*. Cambridge University Press. <https://doi.org/10.1017/9781108846998>
- Ionescu, D., Penno, S., Haimovich, M., Rihtman, B., Goodwin, A., Schwartz, D., et al. (2009). Archaea in the Gulf of Aqaba. *FEMS Microbiology Ecology*, 69(3), 425–438. <https://doi.org/10.1111/j.1574-6941.2009.00721.x>
- Iverson, V., Morris, R. M., Frazar, C. D., Berthiaume, C. T., Morales, R. L., & Armbrust, E. V. (2012). Untangling genomes from metagenomes: Revealing an uncultured class of marine euryarchaeota. *Science*, 335(6068), 587–590. <https://doi.org/10.1126/science.1212665>
- Jaeschke, A., Eickmann, B., Lang, S. Q., Bernasconi, S. M., Strauss, H., & Früh-Green, G. L. (2014). Biosignatures in chimney structures and sediment from the Loki's Castle low-temperature hydrothermal vent field at the Arctic Mid-Ocean Ridge. *Extremophiles*, 18(3), 545–560. <https://doi.org/10.1007/s00792-014-0640-2>
- Jaeschke, A., Jørgensen, S. L., Bernasconi, S. M., Pedersen, R. B., Thorseth, I. H., & Früh-Green, G. L. (2012). Microbial diversity of Loki's Castle black smokers at the Arctic Mid-Ocean Ridge. *Geobiology*, 10(6), 548–561.
- Jaeschke, A., Wengler, M., Hefter, J., Ronge, T. A., Geibert, W., Mollenhauer, G., et al. (2017). A biomarker perspective on dust, productivity, and sea surface temperature in the Pacific sector of the Southern Ocean. *Geochimica et Cosmochimica Acta*, 204, 120–139. <https://doi.org/10.1016/j.gca.2017.01.045>
- Jain, S. (2014). Biosynthesis of archaeal membrane ether lipids. *Frontiers in Microbiology*, 5, 641. <https://doi.org/10.3389/fmicb.2014.00641>
- Jain, S., Caforio, A., Fodran, P., Lolkema, J. S., Minnaard, A. J., & Driessen, A. J. M. (2014). Identification of CDP-archaeol synthase, a missing link of ether lipid biosynthesis in Archaea. *Chemistry & Biology*, 21(10), 1392–1401. <https://doi.org/10.1016/j.chembiol.2014.07.022>
- Jenkyns, H. C., Forster, A., Schouten, S., & Sinninghe Damsté, J. S. (2004). High temperatures in the Late Cretaceous Arctic Ocean. *Nature*, 432(7019), 888–892. <https://doi.org/10.1038/nature03143>
- Jenkyns, H. C., Schouten-Huibers, L., Schouten, S., & Sinninghe Damsté, J. S. (2012). Warm Middle Jurassic–Early Cretaceous high-latitude sea-surface temperatures from the Southern Ocean. *Climate of the Past*, 8(1), 215–226. <https://doi.org/10.5194/cp-8-215-2012>
- Jia, G., Wang, X., Guo, W., & Dong, L. (2017). Seasonal distribution of archaeal lipids in surface water and its constraint on their sources and the TEX_{86} temperature proxy in sediments of the South China Sea. *Journal of Geophysical Research: Biogeosciences*, 122(3), 592–606. <https://doi.org/10.1002/2016jg003732>
- Judd, E. J., Tierney, J. E., Huber, B. T., Wing, S. L., Lunt, D. J., Ford, H. L., et al. (2022). The PhanSST global database of Phanerozoic sea surface temperature proxy data. *Scientific Data*, 9(1), 753. <https://doi.org/10.1038/s41597-022-01826-0>
- Judd, E. J., Tierney, J. E., Lunt, D. J., Montañez, I. P., Huber, B. T., Wing, S. L., & Valdes, P. J. (2024). A 485-million-year history of Earth's surface temperature. *Science*, 385(6715), eadk3705. <https://doi.org/10.1126/science.adk3705>
- Junium, C. K., Meyers, S. R., & Arthur, M. A. (2018). Nitrogen cycle dynamics in the Late Cretaceous Greenhouse. *Earth and Planetary Science Letters*, 481, 404–411. <https://doi.org/10.1016/j.epsl.2017.10.006>
- Kabel, K., Moros, M., Porsche, C., Neumann, T., Adolph, F., Andersen, T. J., et al. (2012). Impact of climate change on the Baltic Sea ecosystem over the past 1,000 years. *Nature Climate Change*, 2(12), 871–874. <https://doi.org/10.1038/nclimate1595>

- Kaiser, J., & Arz, H. W. (2016). Sources of sedimentary biomarkers and proxies with potential paleoenvironmental significance for the Baltic Sea. *Continental Shelf Research*, 122, 102–119. <https://doi.org/10.1016/j.csr.2016.03.020>
- Kaiser, J., Schouten, S., Kilian, R., Arz, H. W., Lamy, F., & Sinninghe Damsté, J. S. (2015). Isoprenoid and branched GDGT-based proxies for surface sediments from marine, fjord and lake environments in Chile. *Organic Geochemistry*, 89–90, 117–127. <https://doi.org/10.1016/j.orggeochem.2015.10.007>
- Kakinuma, K., Obata, Y., Matsuzawa, T., Uzawa, T., & Oshima, T. (1990). The stereochemical fate of glycerol during the biosynthesis of membrane lipids in thermoacidophilic archaeobacteria *Sulfolobus acidocaldarius*. *Journal of the Chemical Society, Chemical Communications*, 13, 925–927. <https://doi.org/10.1039/C39900000925>
- Kaneko, M., Kitajima, F., & Naraoka, H. (2011). Stable hydrogen isotope measurement of archaeal ether-bound hydrocarbons. *Organic Geochemistry*, 42(2), 166–172. <https://doi.org/10.1016/j.orggeochem.2010.11.002>
- Karner, M. B., DeLong, E. F., & Karl, D. M. (2001). Archaeal dominance in the mesopelagic zone of the Pacific Ocean. *Nature*, 409(6819), 507–510. <https://doi.org/10.1038/35054051>
- Kates, M. (1993). Biology of halophilic bacteria, Part II – Membrane lipids of extreme halophiles biosynthesis, function and evolutionary significance. *Experientia*, 49(12), 1027–1036. <https://doi.org/10.1007/bf01929909>
- Kates, M., & Kushwaha, S. (1978). Biochemistry of the lipids of extremely halophilic bacteria. In S. R. Caplan & M. Ginzburg (Eds.), *Energetics and structure of halophilic microorganisms* (pp. 461–479). Elsevier/North-Holland Biomedical Press.
- Kates, M., Sastry, P. S., & Yengoyan, L. S. (1963). Isolation and characterization of a diether analog of phosphatidyl glycerophosphate from *Halobacterium cutirubrum*. *Biochimica et Biophysica Acta - Specialized Section on Lipids and Related Subjects*, 70, 705–707. [https://doi.org/10.1016/0926-6542\(63\)90108-2](https://doi.org/10.1016/0926-6542(63)90108-2)
- Kates, M., Yengoyan, L. S., & Sastry, P. S. (1965). A diether analog of phosphatidyl glycerophosphate in *Halobacterium cutirubrum*. *Biochimica et Biophysica Acta (BBA) - Lipids and Lipid Metabolism*, 98(2), 252–268. [https://doi.org/10.1016/0005-2760\(65\)90119-0](https://doi.org/10.1016/0005-2760(65)90119-0)
- Katoh, K., & Standley, D. M. (2013). MAFFT multiple sequence alignment software Version 7: Improvements in performance and usability. *Molecular Biology and Evolution*, 30(4), 772–780. <https://doi.org/10.1093/molbev/mst010>
- Keller, K., Kopf, S., McFarlin, J., Maloney, A., Rhim, J. H., Elling, F. J., et al. (2025a). Compound-specific carbon and hydrogen isotope analysis traces archaeal lipid signatures in cold seep marine systems. *Geochimica et Cosmochimica Acta*, 407, 309–321. <https://doi.org/10.1016/j.gca.2025.08.017>
- Keller, K. J., Baum, M. M., Liu, X.-L., Ashing-Giwa, K., Baker, I. R., Blewett, J., & Pearson, A. (2025b). Constraining the sources of archaeal tetraether lipids in multiple cold seep provinces of the Cascadia Margin. *Organic Geochemistry*, 200, 104882. <https://doi.org/10.1016/j.orggeochem.2024.104882>
- Kellermann, M. Y., Wegener, G., Elvert, M., Yoshinaga, M. Y., Lin, Y.-S., Holler, T., et al. (2012). Autotrophy as a predominant mode of carbon fixation in anaerobic methane-oxidizing microbial communities. *Proceedings of the National Academy of Sciences*, 109(47), 19321–19326. <https://doi.org/10.1073/pnas.1208795109>
- Kellermann, M. Y., Yoshinaga, M. Y., Wegener, G., Krukenberg, V., & Hinrichs, K.-U. (2016). Tracing the production and fate of individual archaeal intact polar lipids using stable isotope probing. *Organic Geochemistry*, 95, 13–20. <https://doi.org/10.1016/j.orggeochem.2016.02.004>
- Kharbush, J. J., Allen, A. E., Moustafa, A., Dorrestein, P. C., & Aluwihare, L. I. (2016). Intact polar diacylglycerol biomarker lipids isolated from suspended particulate organic matter accumulating in an ultratoligotrophic water column. *Organic Geochemistry*, 100, 29–41. <https://doi.org/10.1016/j.orggeochem.2016.07.008>
- Kim, B., & Zhang, Y. G. (2022). Methane hydrate dissociation across the Oligocene–Miocene boundary. *Nature Geoscience*, 15(3), 203–209. <https://doi.org/10.1038/s41561-022-00895-5>
- Kim, B., & Zhang, Y. G. (2023). Methane Index: Towards a quantitative archaeal lipid biomarker proxy for reconstructing marine sedimentary methane fluxes. *Geochimica et Cosmochimica Acta*, 354, 74–87. <https://doi.org/10.1016/j.gca.2023.06.008>
- Kim, J.-H., Crosta, X., Michel, E., Schouten, S., Duprat, J., & Sinninghe Damsté, J. S. (2009b). Impact of lateral transport on organic proxies in the Southern Ocean. *Quaternary Research*, 71(2), 246–250. <https://doi.org/10.1016/j.yqres.2008.10.005>
- Kim, J.-H., Crosta, X., Willmott, V., Renssen, H., Bonnin, J., Helmke, P., et al. (2012a). Holocene subsurface temperature variability in the eastern Antarctic continental margin. *Geophysical Research Letters*, 39(6), L06705. <https://doi.org/10.1029/2012gl051157>
- Kim, J.-H., Huguet, C., Zonneveld, K. A. F., Versteegh, G. J. M., Roeder, W., Sinninghe Damsté, J. S., & Schouten, S. (2009a). An experimental field study to test the stability of lipids used for the TEX₈₆ and palaeothermometers. *Geochimica et Cosmochimica Acta*, 73(10), 2888–2898. <https://doi.org/10.1016/j.gca.2009.02.030>
- Kim, J.-H., Ludwig, W., Schouten, S., Kerhervé, P., Herfort, L., Bonnin, J., & Sinninghe Damsté, J. S. (2007). Impact of flood events on the transport of terrestrial organic matter to the ocean: A study of the Têt River (SW France) using the BIT index. *Organic Geochemistry*, 38(10), 1593–1606. <https://doi.org/10.1016/j.orggeochem.2007.06.010>
- Kim, J.-H., Romero, O. E., Lohmann, G., Donner, B., Laepple, T., Haam, E., & Sinninghe Damsté, J. S. (2012b). Pronounced subsurface cooling of North Atlantic waters off Northwest Africa during Dansgaard-Oeschger interstadials. *Earth and Planetary Science Letters*, 339–340, 95–102. <https://doi.org/10.1016/j.epsl.2012.05.018>
- Kim, J.-H., Schouten, S., Hopmans, E. C., Donner, B., & Sinninghe Damsté, J. S. (2008). Global sediment core-top calibration of the TEX₈₆ paleothermometer in the ocean. *Geochimica et Cosmochimica Acta*, 72(4), 1154–1173. <https://doi.org/10.1016/j.gca.2007.12.010>
- Kim, J.-H., Schouten, S., Rodrigo-Gámiz, M., Rampen, S., Marino, G., Huguet, C., et al. (2015). Influence of deep-water derived isoprenoid tetraether lipids on the TEX₈₆^H paleothermometer in the Mediterranean Sea. *Geochimica et Cosmochimica Acta*, 150, 125–141. <https://doi.org/10.1016/j.gca.2014.11.017>
- Kim, J.-H., van der Meer, J., Schouten, S., Helmke, P., Willmott, V., Sangiorgi, F., et al. (2010). New indices and calibrations derived from the distribution of crenarchaeal isoprenoid tetraether lipids: Implications for past sea surface temperature reconstructions. *Geochimica et Cosmochimica Acta*, 74(16), 4639–4654. <https://doi.org/10.1016/j.gca.2010.05.027>
- Kim, J.-H., Villanueva, L., Zell, C., & Sinninghe Damsté, J. S. (2016). Biological source and provenance of deep-water derived isoprenoid tetraether lipids along the Portuguese continental margin. *Geochimica et Cosmochimica Acta*, 172, 177–204. <https://doi.org/10.1016/j.gca.2015.09.010>
- Knappy, C. S., Barillà, D., Chong, J., Hodgson, D., Morgan, H., Suleman, M., et al. (2015). Mono-di- and trimethylated homologues of isoprenoid tetraether lipid cores in archaea and environmental samples: Mass spectrometric identification and significance. *Journal of Mass Spectrometry*, 50(12), 1420–1432. <https://doi.org/10.1002/jms.3709>
- Knappy, C. S., & Keely, B. J. (2012). Novel glycerol dialkanol triols in sediments: Transformation products of glycerol dibiphytanyl glycerol tetraether lipids or biosynthetic intermediates? *Chemical Communications*, 48(6), 841–843. <https://doi.org/10.1039/c1cc15841d>
- Knappy, C. S., Yao, P., Pickering, M. D., & Keely, B. J. (2014). Identification of homoglycerol- and dihomoglycerol-containing isoprenoid tetraether lipid cores in aquatic sediments and a soil. *Organic Geochemistry*, 76, 146–156. <https://doi.org/10.1016/j.orggeochem.2014.06.003>

- Knittel, K., & Boetius, A. (2009). Anaerobic Oxidation of Methane: Progress with an Unknown Process. *Annual Review of Microbiology*, 63(1), 311–334. <https://doi.org/10.1146/annurev.micro.61.080706.093130>
- Koga, Y., Akagawa-Matsushita, M., Ohga, M., & Nishihara, M. (1993b). Taxonomic significance of the distribution of component parts of polar ether lipids in methanogens. *Systematic and Applied Microbiology*, 16(3), 342–351. [https://doi.org/10.1016/s0723-2020\(11\)80264-x](https://doi.org/10.1016/s0723-2020(11)80264-x)
- Koga, Y., & Morii, H. (2005). Recent advances in structural research on ether lipids from archaea including comparative and physiological aspects. *Bioscience, Biotechnology, and Biochemistry*, 69(11), 2019–2034. <https://doi.org/10.1271/bbb.69.2019>
- Koga, Y., & Morii, H. (2007). Biosynthesis of ether-type polar lipids in archaea and evolutionary considerations. *Microbiology and Molecular Biology Reviews*, 71(1), 97–120. <https://doi.org/10.1128/mmb.00033-06>
- Koga, Y., Nishihara, M., Morii, H., & Akagawa-Matsushita, M. (1993a). Ether polar lipids of methanogenic bacteria: Structures, comparative aspects, and biosyntheses. *Microbiological Reviews*, 57(1), 164–182. <https://doi.org/10.1128/mr.57.1.164-182.1993>
- Könneke, M., Bernhard, A. E., de la Torre, J. R., Walker, C. B., Waterbury, J. B., & Stahl, D. A. (2005). Isolation of an autotrophic ammonia-oxidizing marine archaeon. *Nature*, 437(7058), 543–546. <https://doi.org/10.1038/nature03911>
- Könneke, M., Lipp, J. S., & Hinrichs, K.-U. (2012). Carbon isotope fractionation by the marine ammonia-oxidizing archaeon *Nitrosopumilus maritimus*. *Organic Geochemistry*, 48, 21–24. <https://doi.org/10.1016/j.orggeochem.2012.04.007>
- Könneke, M., Schubert, D. M., Brown, P. C., Hugler, M., Standfest, S., Schwander, T., et al. (2014). Ammonia-oxidizing archaea use the most energy-efficient aerobic pathway for CO₂ fixation. *Proceedings of the National Academy of Sciences*, 111(22), 8239–8244. <https://doi.org/10.1073/pnas.1402028111>
- Kremer, A., Stein, R., Fahl, K., Ji, Z., Yang, Z., Wiers, S., et al. (2018). Changes in sea ice cover and ice sheet extent at the Yermak Plateau during the last 160 ka – Reconstructions from biomarker records. *Quaternary Science Reviews*, 182, 93–108. <https://doi.org/10.1016/j.quascirev.2017.12.016>
- Kropp, C., Lipp, J., Schmidt, A. L., Seisenberger, C., Linde, M., Hinrichs, K., & Babinger, P. (2022). Identification of acetylated diether lipids in halophilic Archaea. *MicrobiologyOpen*, 11(3), e1299. <https://doi.org/10.1002/mbo3.1299>
- Kurth, J. M., Smit, N. T., Berger, S., Schouten, S., Jetten, M. S. M., & Welte, C. U. (2019). Anaerobic methanotrophic archaea of the ANME-2d clade feature lipid composition that differs from other ANME archaea. *FEMS Microbiology Ecology*, 95(7), f082. <https://doi.org/10.1093/femsec/fiz082>
- Kusch, S., Rethemeyer, J., Hopmans, E. C., Wacker, L., & Mollenhauer, G. (2016). Factors influencing ¹⁴C concentrations of algal and archaeal lipids and their associated sea surface temperature proxies in the Black Sea. *Geochimica et Cosmochimica Acta*, 188, 35–57. <https://doi.org/10.1016/j.gca.2016.05.025>
- Kuypers, M. M. M., Blokker, P., Erbacher, Kinkel, H., Pancost, R. D., Schouten, S., & Sinninghe Damsté, J. S. (2001). Massive expansion of marine archaea during a mid-Cretaceous oceanic anoxic event. *Science*, 293(5527), 92–95. <https://doi.org/10.1126/science.1058424>
- Kuypers, M. M. M., Blokker, P., Hopmans, E. C., Kinkel, H., Pancost, R. D., Schouten, S., & Sinninghe Damsté, J. S. (2002). Archaeal remains dominate marine organic matter from the early Albian oceanic anoxic event 1b. *Palaeogeography, Palaeoclimatology, Palaeoecology*, 185(1–2), 211–234. [https://doi.org/10.1016/s0031-0182\(02\)00301-2](https://doi.org/10.1016/s0031-0182(02)00301-2)
- Labrenz, M., Sintes, E., Toetzk, F., Zumsteg, A., Herndl, G. J., Seidler, M., & Jürgens, K. (2010). Relevance of a crenarchaeotal subcluster related to *Candidatus Nitrosopumilus maritimus* to ammonia oxidation in the suboxic zone of the central Baltic Sea. *The ISME Journal*, 4(12), 1496–1508. <https://doi.org/10.1038/ismej.2010.78>
- Lam, P., Jensen, M. M., Lavik, G., McGinnis, D. F., Muller, B., Schubert, C. J., et al. (2007). Linking crenarchaeal and bacterial nitrification to anammox in the Black Sea. *Proceedings of the National Academy of Sciences*, 104(17), 7104–7109. <https://doi.org/10.1073/pnas.0611081104>
- Lam, P., & Kuypers, M. M. M. (2011). Microbial Nitrogen Cycling Processes in Oxygen Minimum Zones. *Annual Review of Marine Science*, 3(1), 317–345. <https://doi.org/10.1146/annurev-marine-120709-142814>
- Lamping, N., Müller, J., Hefter, J., Mollenhauer, G., Haas, C., Shi, X., et al. (2021). Evaluation of lipid biomarkers as proxies for sea ice and ocean temperatures along the Antarctic continental margin. *Climate of the Past*, 17(5), 2305–2326. <https://doi.org/10.5194/cp-17-2305-2021>
- Langworthy, T. A. (1977). Long-chain diglycerol tetraethers from *Thermoplasma acidophilum*. *Biochimica et Biophysica Acta (BBA) - Lipids and Lipid Metabolism*, 487(1), 37–50. [https://doi.org/10.1016/0005-2760\(77\)90042-X](https://doi.org/10.1016/0005-2760(77)90042-X)
- Langworthy, T. A., Tornabene, T. G., & Holzer, G. (1982). Lipids of archaebacteria. *Zbl. Bakt. Hyg., I. Abt. Orig. C*, 3(2), 228–244. [https://doi.org/10.1016/s0721-9571\(82\)80036-7](https://doi.org/10.1016/s0721-9571(82)80036-7)
- Law, K. P., He, W., Tao, J., & Zhang, C. (2021). A novel approach to characterize the lipidome of marine archaeon *Nitrosopumilus maritimus* by ion mobility mass spectrometry. *Frontiers in Microbiology*, 12, 735878. <https://doi.org/10.3389/fmicb.2021.735878>
- Lawrence, K. T., Pearson, A., Castañeda, I. S., Ladlow, C., Peterson, L. C., & Lawrence, C. E. (2020). Comparison of late Neogene U^k₃₇ and TEX₈₆ paleotemperature records from the eastern equatorial Pacific at orbital resolution. *Paleoceanography and Paleoclimatology*, 35(7), e2020PA003858. <https://doi.org/10.1029/2020pa003858>
- Leavitt, W. D., Kopf, S. H., Weber, Y., Chiu, B., McFarlin, J. M., Elling, F. J., et al. (2023). Controls on the hydrogen isotope composition of tetraether lipids in an autotrophic ammonia-oxidizing marine archaeon. *Geochimica et Cosmochimica Acta*, 352, 194–210. <https://doi.org/10.1016/j.gca.2023.04.033>
- Lengger, S. K., Hopmans, E. C., Reichart, G.-J., Nierop, K. G. J., Sinninghe Damsté, J. S., & Schouten, S. (2012). Intact polar and core glycerol dibiphytanyl glycerol tetraether lipids in the Arabian Sea oxygen minimum zone. Part II: Selective preservation and degradation in sediments and consequences for the TEX₈₆. *Geochimica et Cosmochimica Acta*, 98, 244–258. <https://doi.org/10.1016/j.gca.2012.05.003>
- Lengger, S. K., Hopmans, E. C., Sinninghe Damsté, J. S., & Schouten, S. (2014a). Impact of sedimentary degradation and deep water column production on GDGT abundance and distribution in surface sediments in the Arabian Sea: Implications for the TEX₈₆ paleothermometer. *Geochimica et Cosmochimica Acta*, 142, 386–399. <https://doi.org/10.1016/j.gca.2014.07.013>
- Lengger, S. K., Kraaij, M., Tjallingii, R., Baas, M., Stuut, J.-B., Hopmans, E. C., et al. (2013). Differential degradation of intact polar and core glycerol dialkyl glycerol tetraether lipids upon post-depositional oxidation. *Organic Geochemistry*, 65, 83–93. <https://doi.org/10.1016/j.orggeochem.2013.10.004>
- Lengger, S. K., Lipsewiers, Y. A., de Haas, H., Sinninghe Damsté, J. S., & Schouten, S. (2014b). Lack of ¹³C-label incorporation suggests low turnover rates of thaumarchaeal intact polar tetraether lipids in sediments from the Iceland shelf. *Biogeosciences*, 11(2), 201–216. <https://doi.org/10.5194/bg-11-201-2014>
- Lengger, S. K., Weber, Y., Taylor, K. W. R., Kopf, S. H., Berstan, R., Bull, I. D., et al. (2021). Determination of the δ²H values of high molecular weight lipids by high-temperature gas chromatography coupled to isotope ratio mass spectrometry. *Rapid Communications in Mass Spectrometry*, 35(4), e8983. <https://doi.org/10.1002/rcm.8983>
- Levitus, S., Boyer, T. P., Conkright, M. E., O'Brien, T., Antonov, J., Stephens, C., et al. (1998). World ocean database 1998 (Vol. 1).
- Li, F., Leu, A., Poff, K., Carlson, L. T., Ingalls, A. E., & DeLong, E. F. (2021). Planktonic archaeal ether lipid origins in surface waters of the North Pacific subtropical gyre. *Frontiers in Microbiology*, 12, 610675. <https://doi.org/10.3389/fmicb.2021.610675>

- Li, Y., Yu, T., Feng, X., Zhao, B., Chen, H., Yang, H., et al. (2024). Biosynthesis of GMDT lipids by a radical SAM enzyme associated with anaerobic archaea and oxygen-deficient environments. *Nature Communications*, 15(1), 5256. <https://doi.org/10.1038/s41467-024-49650-x>
- Lin, Y.-S., Lipp, J. S., Elvert, M., Holler, T., & Hinrichs, K.-U. (2013). Assessing production of the ubiquitous archaeal diglycosyl tetraether lipids in marine subsurface sediment using intramolecular stable isotope probing: Stable isotope probing of 2G-GDGTs. *Environmental Microbiology*, 15(5), 1634–1646. <https://doi.org/10.1111/j.1462-2920.2012.02888.x>
- Lin, Y.-S., Lipp, J. S., Yoshinaga, M. Y., Lin, S.-H., Elvert, M., & Hinrichs, K.-U. (2010). Intramolecular stable carbon isotopic analysis of archaeal glycosyl tetraether lipids. *Rapid Communications in Mass Spectrometry*, 24(19), 2817–2826. <https://doi.org/10.1002/rcm.4707>
- Lincoln, S. A., Bradley, A. S., Newman, S. A., & Summons, R. E. (2013). Archaeal and bacterial glycerol dialkyl glycerol tetraether lipids in chimneys of the Lost City Hydrothermal Field. *Organic Geochemistry*, 60, 45–53. <https://doi.org/10.1016/j.orggeochem.2013.04.010>
- Lincoln, S. A., Wai, B., Eppley, J. M., Church, M. J., Summons, R. E., & DeLong, E. F. (2014a). Planktonic Euryarchaeota are a significant source of archaeal tetraether lipids in the ocean. *Proceedings of the National Academy of Sciences*, 111(27), 9858–9863. <https://doi.org/10.1073/pnas.1409439111>
- Lincoln, S. A., Wai, B., Eppley, J. M., Church, M. J., Summons, R. E., & DeLong, E. F. (2014b). Reply to Schouten et al.: Marine Group II planktonic Euryarchaeota are significant contributors to tetraether lipids in the ocean. *Proceedings of the National Academy of Sciences*, 111(41), E4286. <https://doi.org/10.1073/pnas.1416736111>
- Linnert, C., Robinson, S. A., Lees, J. A., Bown, P. R., Pérez-Rodríguez, I., Petrizzo, M. R., et al. (2014). Evidence for global cooling in the Late Cretaceous. *Nature Communications*, 5(1), 4194. <https://doi.org/10.1038/ncomms5194>
- Lipp, J. S., & Hinrichs, K.-U. (2009). Structural diversity and fate of intact polar lipids in marine sediments. *Geochimica et Cosmochimica Acta*, 73(22), 6816–6833. <https://doi.org/10.1016/j.gca.2009.08.003>
- Littler, K., Robinson, S. A., & Bown, P. R. (2014). An offset in TEX₈₆ values between interbedded lithologies: Implications for sea-surface temperature reconstructions. *Paleogeography, Palaeoclimatology, Palaeoecology*, 399, 42–51. <https://doi.org/10.1016/j.palaeo.2014.02.009>
- Littler, K., Robinson, S. A., Bown, P. R., Nederbragt, A. J., & Pancost, R. D. (2011). High sea-surface temperatures during the Early Cretaceous Epoch. *Nature Geoscience*, 4(3), 169–172. <https://doi.org/10.1038/ngeo1081>
- Liu, X., Lipp, J. S., & Hinrichs, K.-U. (2011). Distribution of intact and core GDGTs in marine sediments. *Organic Geochemistry*, 42(4), 368–375. <https://doi.org/10.1016/j.orggeochem.2011.02.003>
- Liu, X.-L., Birgel, D., Elling, F. J., Sutton, P. A., Lipp, J. S., Zhu, R., et al. (2016). From ether to acid: A plausible degradation pathway of glycerol dialkyl glycerol tetraethers. *Geochimica et Cosmochimica Acta*, 183, 138–152. <https://doi.org/10.1016/j.gca.2016.04.016>
- Liu, X.-L., Lipp, J. S., Birgel, D., Summons, R. E., & Hinrichs, K.-U. (2018). Predominance of parallel glycerol arrangement in archaeal tetraethers from marine sediments: Structural features revealed from degradation products. *Organic Geochemistry*, 115, 12–23. <https://doi.org/10.1016/j.orggeochem.2017.09.009>
- Liu, X.-L., Lipp, J. S., Schröder, J. M., Summons, R. E., & Hinrichs, K.-U. (2012b). Isoprenoid glycerol dialkanol diethers: A series of novel archaeal lipids in marine sediments. *Organic Geochemistry*, 43, 50–55. <https://doi.org/10.1016/j.orggeochem.2011.11.002>
- Liu, X.-L., Lipp, J. S., Simpson, J. H., Lin, Y.-S., Summons, R. E., & Hinrichs, K.-U. (2012c). Mono- and dihydroxyl glycerol dibiphytanyl glycerol tetraethers in marine sediments: Identification of both core and intact polar lipid forms. *Geochimica et Cosmochimica Acta*, 89, 102–115. <https://doi.org/10.1016/j.gca.2012.04.053>
- Liu, X.-L., Russell, D. A., Bonfio, C., & Summons, R. E. (2019). Glycerol configurations of environmental GDGTs investigated using a selective sn2 ether cleavage protocol. *Organic Geochemistry*, 128, 57–62. <https://doi.org/10.1016/j.orggeochem.2018.12.003>
- Liu, X.-L., Summons, R. E., & Hinrichs, K.-U. (2012a). Extending the known range of glycerol ether lipids in the environment: Structural assignments based on tandem mass spectral fragmentation patterns: Extending the known range of glycerol ether lipids in the environment. *Rapid Communications in Mass Spectrometry*, 26(19), 2295–2302. <https://doi.org/10.1002/rcm.6355>
- Liu, X.-L., Zhu, C., Wakeham, S. G., & Hinrichs, K.-U. (2014). In situ production of branched glycerol dialkyl glycerol tetraethers in anoxic marine water columns. *Marine Chemistry*, 166, 1–8. <https://doi.org/10.1016/j.marchem.2014.08.008>
- Liu, Z., Pagani, M., Zinniker, D., DeConto, R., Huber, M., Brinkhuis, H., et al. (2009). Global Cooling During the Eocene-Oligocene Climate Transition. *Science*, 323(5918), 1187–1190. <https://doi.org/10.1126/science.1166368>
- Lloyd, C. T., Iwig, D. F., Wang, B., Cossu, M., Metcalf, W. W., Boal, A. K., & Booker, S. J. (2022). Discovery, structure and mechanism of a tetraether lipid synthase. *Nature*, 609(7925), 197–203. <https://doi.org/10.1038/s41586-022-05120-2>
- Lo, L., Belt, S. T., Lattaud, J., Friedrich, T., Zeeden, C., Schouten, S., et al. (2018). Precession and atmospheric CO₂ modulated variability of sea ice in the central Okhotsk Sea since 130,000 years ago. *Earth and Planetary Science Letters*, 488, 36–45. <https://doi.org/10.1016/j.epsl.2018.02.005>
- Locarnini, R. A., Mishonov, A. V., Baranova, O. K., Boyer, T. P., Zweng, M. M., Garcia, H. E., et al. (2019). Volume 1: Temperature. *World Ocean Atlas 2018*.
- Locarnini, R. A., Mishonov, A. V., Baranova, O. K., Reagan, J. R., Boyer, T. P., Seidov, D., et al. (2024). Volume 1: Temperature. *World Ocean Atlas 2023*. <https://doi.org/10.25923/54BH-1613>
- Logemann, J., Graue, J., Köster, J., Engelen, B., Rullkötter, J., & Cypionka, H. (2011). A laboratory experiment of intact polar lipid degradation in sandy sediments. *Biogeosciences*, 8(9), 2547–2560. <https://doi.org/10.5194/bg-8-2547-2011>
- Lopes dos Santos, R. A., Prange, M., Castañeda, I. S., Schefuß, E., Mulitz, S., Schulz, M., et al. (2010). Glacial–interglacial variability in Atlantic meridional overturning circulation and thermocline adjustments in the tropical North Atlantic. *Earth and Planetary Science Letters*, 300(3–4), 407–414. <https://doi.org/10.1016/j.epsl.2010.10.030>
- Lopes dos Santos, R. A., Spooner, M. I., Barrows, T. T., De Deckker, P., Sinninghe Damsté, J. S., & Schouten, S. (2013). Comparison of organic (U^K₃₇, TEX₈₆^H, LDI) and faunal proxies (foraminiferal assemblages) for reconstruction of late Quaternary sea surface temperature variability from offshore southeastern Australia. *Paleoceanography*, 28(3), 377–387. <https://doi.org/10.1002/palo.20035>
- López-García, P., Moreira, D., López-López, A., & Rodríguez-Valera, F. (2001). A novel haloarchaeal-related lineage is widely distributed in deep oceanic regions. *Environmental Microbiology*, 3(1), 72–78. <https://doi.org/10.1046/j.1462-2920.2001.00162.x>
- Lü, X., Liu, X.-L., Elling, F. J., Yang, H., Xie, S., Song, J., et al. (2015). Hydroxylated isoprenoid GDGTs in Chinese coastal seas and their potential as a paleotemperature proxy for mid-to-low latitude marginal seas. *Organic Geochemistry*, 89–90, 31–43. <https://doi.org/10.1016/j.orggeochem.2015.10.004>
- Lu, Y., Xia, X., Cheung, S., Jing, H., & Liu, H. (2019). Differential distribution and determinants of ammonia oxidizing archaea sublineages in the oxygen minimum zone off Costa Rica. *Microorganisms*, 7(10), 453. <https://doi.org/10.3390/microorganisms7100453>
- Lutnaes, B. F., Krane, J., Smith, B. E., & Rowland, S. J. (2007). Structure elucidation of C80, C81 and C82 isoprenoid tetraacids responsible for naphthenate deposition in crude oil production. *Organic & Biomolecular Chemistry*, 5(12), 1873–1877. <https://doi.org/10.1039/B701462G>
- Ma, C., Coffinet, S., Lipp, J. S., Hinrichs, K.-U., & Zhang, C. (2020). Marine group II Euryarchaeota contribute to the archaeal lipid pool in northwestern Pacific Ocean surface waters. *Frontiers in Microbiology*, 11, 1034. <https://doi.org/10.3389/fmicb.2020.01034>

- Martijn, J., Schön, M. E., Lind, A. E., Vosseberg, J., Williams, T. A., Spang, A., & Ettema, T. J. G. (2020). Hikarchaeia demonstrate an intermediate stage in the methanogen-to-halophile transition. *Nature Communications*, 11(1), 5490. <https://doi.org/10.1038/s41467-020-19200-2>
- Martin, J. H., Knauer, G. A., Karl, D. M., & Broenkow, W. W. (1987). VERTEX: Carbon cycling in the northeast Pacific. *Deep-Sea Research, Part A: Oceanographic Research Papers*, 34(2), 267–285. [https://doi.org/10.1016/0198-0149\(87\)90086-0](https://doi.org/10.1016/0198-0149(87)90086-0)
- Martin-Cuadrado, A.-B., Garcia-Heredia, I., Moltó, A. G., López-Úbeda, R., Kimes, N., López-García, P., et al. (2015). A new class of marine Euryarchaeota group II from the mediterranean deep chlorophyll maximum. *The ISME Journal*, 9(7), 1619–1634. <https://doi.org/10.1038/ismej.2014.249>
- Martínez-Sosa, P., Tierney, J. E., Pérez-Angel, L. C., Stefanescu, I. C., Guo, J., Kirkels, F., et al. (2023). Development and application of the branched and isoprenoid GDGT machine learning classification algorithm (BIGMaC) for paleoenvironmental reconstruction. *Paleoceanography and Paleoclimatology*, 38(7), e2023PA004611. <https://doi.org/10.1029/2023PA004611>
- Massana, R., DeLong, E. F., & Pedros-Alio, C. (2000). A few cosmopolitan phylotypes dominate planktonic archaeal assemblages in widely different oceanic provinces. *Applied and Environmental Microbiology*, 66(5), 1777–1787. <https://doi.org/10.1128/aem.66.5.1777-1787.2000>
- Matsumi, R., Atomi, H., Driessen, A. J. M., & van der Oost, J. (2011). Isoprenoid biosynthesis in Archaea – Biochemical and evolutionary implications. *Research in Microbiology*, 162(1), 39–52. <https://doi.org/10.1016/j.resmic.2010.10.003>
- McClymont, E. L., Ganeshram, R. S., Pichevin, L. E., Talbot, H. M., van Dongen, B. E., Thunell, R. C., et al. (2012). Sea-surface temperature records of Termination 1 in the Gulf of California: Challenges for seasonal and interannual analogues of tropical Pacific climate change. *Paleoceanography*, 27(2), PA2202. <https://doi.org/10.1029/2011pa002226>
- Meador, T. B., Bowles, M., Lazar, C. S., Zhu, C., Teske, A., & Hinrichs, K.-U. (2015). The archaeal lipidome in estuarine sediment dominated by members of the Miscellaneous Crenarchaeotal Group. *Environmental Microbiology*, 17(7), 2441–2458. <https://doi.org/10.1111/1462-2920.12716>
- Meador, T. B., Zhu, C., Elling, F. J., Könneke, M., & Hinrichs, K.-U. (2014). Identification of isoprenoid glycosidic glycerol dibiphytanol diethers and indications for their biosynthetic origin. *Organic Geochemistry*, 69, 70–75. <https://doi.org/10.1016/j.orggeochem.2014.02.005>
- Mekik, F., & Anderson, R. (2018). Is the core top modern? Observations from the eastern equatorial Pacific. *Quaternary Science Reviews*, 186, 156–168. <https://doi.org/10.1016/j.quascirev.2018.01.020>
- Menzel, D., Hopmans, E. C., Schouten, S., & Sinninghe Damsté, J. S. (2006). Membrane tetraether lipids of planktonic Crenarchaeota in Pliocene sapropels of the eastern Mediterranean Sea. *Palaeogeography, Palaeoclimatology, Palaeoecology*, 239(1–2), 1–15. <https://doi.org/10.1016/j.palaeo.2006.01.002>
- Meunier-Christmann, C. (1988). *Geochimie organique de phosphates et schistes bitumineux marocains: etude du processus de phosphatogenese* (PhD Thesis). Université de Strasbourg. Retrieved from <https://theses.fr/1988STR13200>
- Meyer, V. D., Max, L., Hefter, J., Tiedemann, R., & Mollenhauer, G. (2016). Glacial-to-Holocene evolution of sea surface temperature and surface circulation in the subarctic northwest Pacific and the Western Bering Sea. *Paleoceanography*, 31(7), 916–927. <https://doi.org/10.1002/2015PA002877>
- Millero, F. J. (1995). Thermodynamics of the carbon dioxide system in the oceans. *Geochimica et Cosmochimica Acta*, 59(4), 661–677. [https://doi.org/10.1016/0016-7037\(94\)00354-O](https://doi.org/10.1016/0016-7037(94)00354-O)
- Moldowan, J. M., & Seifert, W. K. (1979). Head-to-Head Linked Isoprenoid Hydrocarbons in Petroleum. *Science*, 204(4389), 169–171. <https://doi.org/10.1126/science.204.4389.169>
- Mollenhauer, G., Basse, A., Kim, J.-H., Sinninghe Damsté, J. S., & Fischer, G. (2015). A four-year record of $U^{K'}$ - and TEX_{86} -derived sea surface temperature estimates from sinking particles in the filamentous upwelling region off Cape Blanc, Mauritania. *Deep Sea Research Part I: Oceanographic Research Papers*, 97, 67–79. <https://doi.org/10.1016/j.dsr.2014.11.015>
- Mollenhauer, G., Eglinton, T. I., Hopmans, E. C., & Sinninghe Damsté, J. S. (2008). A radiocarbon-based assessment of the preservation characteristics of crenarchaeol and alkenones from continental margin sediments. *Organic Geochemistry*, 39(8), 1039–1045. <https://doi.org/10.1016/j.orggeochem.2008.02.006>
- Mollenhauer, G., Inthorn, M., Vogt, T., Zabel, M., Sinninghe Damsté, J. S., & Eglinton, T. I. (2007). Aging of marine organic matter during cross-shelf lateral transport in the Benguela upwelling system revealed by compound-specific radiocarbon dating. *Geochemistry, Geophysics, Geosystems*, 8(9), Q09004. <https://doi.org/10.1029/2007GC001603>
- Morillo-Montalbá, L., Rodrigo-Gámiz, M., Martínez-Ruiz, F., Ortega-Huertas, M., Schouten, S., & Sinninghe Damsté, J. S. (2021). Rapid climate changes in the Westernmost Mediterranean (Alboran Sea) over the last 35 kyr: New insights from four lipid paleothermometers ($U^{K'}$, TEX_{86} , RI-OH, and LDI). *Paleoceanography and Paleoclimatology*, 36(12), e2020PA004171. <https://doi.org/10.1029/2020PA004171>
- Mori, T., Isobe, K., Ogawa, T., Yoshimura, T., & Hemmi, H. (2015). A phytoene desaturase homolog gene from the methanogenic archaeon *Methanosarcina acetivorans* is responsible for hydroxyarchaeol biosynthesis. *Biochemical and Biophysical Research Communications*, 466(2), 186–191. <https://doi.org/10.1016/j.bbrc.2015.09.001>
- Morii, H., Eguchi, T., Nishihara, M., Kakinuma, K., König, H., & Koga, Y. (1998). A novel ether core lipid with H-shaped C80-isoprenoid hydrocarbon chain from the hyperthermophilic methanogen *Methanothermobacter fervidus*. *Biochimica et Biophysica Acta*, 1390(3), 339–345. [https://doi.org/10.1016/S0005-2760\(97\)00183-5](https://doi.org/10.1016/S0005-2760(97)00183-5)
- Morii, H., Kiyonari, S., Ishino, Y., & Koga, Y. (2009). A novel biosynthetic pathway of archaeidyl-myoinositol via archaeidyl-myoinositol Phosphate from CDP-archaeol and d-glucose 6-phosphate in methanoarchaeon *Methanothermobacter thermautotrophicus* Cells. *Journal of Biological Chemistry*, 284(45), 30766–30774. <https://doi.org/10.1074/jbc.M109.034652>
- Morii, H., & Koga, Y. (2003). CDP-2,3-Di-O-Geranylgeranyl-sn-Glycerol:L-Serine O-Archaeidyltransferase (Archaeidylserine Synthase) in the Methanogenic Archaeon *Methanothermobacter thermautotrophicus*. *Journal of Bacteriology*, 185(4), 1181–1189. <https://doi.org/10.1128/jb.185.4.1181-1189.2003>
- Morii, H., Yagi, H., Akutsu, H., Nomura, N., Sako, Y., & Koga, Y. (1999). A novel phosphoglycolipid archaeidyl(glucosyl)inositol with two sesterterpanyl chains from the aerobic hyperthermophilic archaeon *Aeropyrum pernix* K1. *Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipids*, 1436(3), 426–436. [https://doi.org/10.1016/S0005-2760\(98\)00157-X](https://doi.org/10.1016/S0005-2760(98)00157-X)
- Müller, P. J., Kirst, G., Ruhland, G., von Storch, I., & Rosell-Melé, A. (1998). Calibration of the alkenone paleotemperature index $U^{K'}$ based on core-tops from the eastern South Atlantic and the global ocean (60°N–60°S). *Geochimica et Cosmochimica Acta*, 62(10), 1757–1772. [https://doi.org/10.1016/S0016-7037\(98\)00097-0](https://doi.org/10.1016/S0016-7037(98)00097-0)
- Murakami, M., Shibuya, K., Nakayama, T., Nishino, T., Yoshimura, T., & Hemmi, H. (2007). Geranylgeranyl reductase involved in the biosynthesis of archaeal membrane lipids in the hyperthermophilic archaeon *Archaeoglobus fulgidus*: Archaeidic acid-synthesizing archaeal reductase. *FEBS Journal*, 274(3), 805–814. <https://doi.org/10.1111/j.1742-4658.2006.05625.x>
- Mutterlose, J., Malkoc, M., Schouten, S., Sinninghe Damsté, J. S., & Forster, A. (2010). TEX_{86} and stable $\delta^{18}O$ paleothermometry of early Cretaceous sediments: Implications for belemnite ecology and paleotemperature proxy application. *Earth and Planetary Science Letters*, 298(3), 286–298. <https://doi.org/10.1016/j.epsl.2010.07.043>

- Naafs, B. D. A., & Pancost, R. D. (2016). Sea-surface temperature evolution across Aptian Oceanic Anoxic Event 1a. *Geology*, 44(11), 959–962. <https://doi.org/10.1130/G38575.1>
- Naafs, B. D. A., Rohrsen, M., Inglis, G. N., Lähteenoja, O., Feakins, S. J., Collinson, M. E., et al. (2018). High temperatures in the terrestrial mid-latitudes during the early Palaeogene. *Nature Geoscience*, 11(10), 766–771. <https://doi.org/10.1038/s41561-018-0199-0>
- Naafs, B. D. A., Voelker, A. H. L., Karas, C., Andersen, N., & Sierro, F. J. (2020). Repeated near-collapse of the Pliocene sea surface temperature gradient in the North Atlantic. *Paleoceanography and Paleoclimatology*, 35(5), e2020PA003905. <https://doi.org/10.1029/2020PA003905>
- Naeher, S., Niemann, H., Peterse, F., Smittenberg, R. H., Ziegler, P. K., & Schubert, C. J. (2014). Tracing the methane cycle with lipid biomarkers in Lake Rotsee (Switzerland). *Organic Geochemistry*, 66, 174–181. <https://doi.org/10.1016/j.orggeochem.2013.11.002>
- Napier, T. J., Wörmer, L., Wendt, J., Lückge, A., Rohlf, N., & Hinrichs, K.-U. (2022). Sub-annual to interannual Arabian Sea upwelling, sea surface temperature, and Indian monsoon rainfall reconstructed using congruent micrometer-scale climate proxies. *Paleoceanography and Paleoclimatology*, 37(3), e2021PA004355. <https://doi.org/10.1029/2021PA004355>
- Nemoto, N., Shida, Y., Shimada, H., Oshima, T., & Yamagishi, A. (2003). Characterization of the precursor of tetraether lipid biosynthesis in the thermophilic archaeon *Thermoplasma acidophilum*. *Extremophiles*, 7(3), 235–243. <https://doi.org/10.1007/s00792-003-0315-x>
- Neubauer, C., Kantnerová, K., Lamothe, A., Savarino, J., Hinkert, A., Juchelka, D., et al. (2023). Discovering nature's fingerprints: Isotope ratio analysis on bioanalytical mass spectrometers. *Journal of the American Society for Mass Spectrometry*, 34(4), 525–537. <https://doi.org/10.1021/jasms.2c00363>
- Ngugi, D. K., Blom, J., Alam, I., Rashid, M., Ba-Alawi, W., Zhang, G., et al. (2015). Comparative genomics reveals adaptations of a halotolerant thaumarchaeon in the interfaces of brine pools in the Red Sea. *The ISME Journal*, 9(2), 396–411. <https://doi.org/10.1038/ismej.2014.137>
- Nguyen, L.-T., Schmidt, H. A., von Haeseler, A., & Minh, B. Q. (2015). IQ-TREE: A fast and effective stochastic algorithm for estimating maximum-likelihood phylogenies. *Molecular Biology and Evolution*, 32(1), 268–274. <https://doi.org/10.1093/molbev/msu300>
- Niemann, H., & Elvert, M. (2008). Diagnostic lipid biomarker and stable carbon isotope signatures of microbial communities mediating the anaerobic oxidation of methane with sulphate. *Organic Geochemistry*, 39(12), 1668–1677. <https://doi.org/10.1016/j.orggeochem.2007.11.003>
- Nunoura, T., Takaki, Y., Hirai, M., Shimamura, S., Makabe, A., Koide, O., et al. (2015). Hadal biosphere: Insight into the microbial ecosystem in the deepest ocean on Earth. *Proceedings of the National Academy of Sciences*, 112(11), E1230–E1236. <https://doi.org/10.1073/pnas.1421816112>
- Obrecht, I., Wörmer, L., Varma, D., De Vleeschouwer, D., Schulz, H., Kucera, M., & Hinrichs, K.-U. (2025). Influence of Mediterranean Oceanographic and Environmental Conditions on Molecular Proxy-Based Sea Surface Temperature Reconstructions During the Last Interglacial. *Paleoceanography and Paleoclimatology*, 40(4), e2024PA004951. <https://doi.org/10.1029/2024PA004951>
- O'Brien, C. L., Robinson, S. A., Pancost, R. D., Sinninghe Damsté, J. S., Schouten, S., Lunt, D. J., et al. (2017). Cretaceous sea-surface temperature evolution: Constraints from TEX₈₆ and planktonic foraminiferal oxygen isotopes. *Earth-Science Reviews*, 172, 224–247. <https://doi.org/10.1016/j.earscirev.2017.07.012>
- Oren, A. (2024). On validly published names, correct names, and changes in the nomenclature of phyla and genera of prokaryotes: A guide for the perplexed. *Npj Biofilms and Microbiomes*, 10(1), 20. <https://doi.org/10.1038/s41522-024-00494-9>
- Oren, A., & Garrity, G. M. (2021). Valid publication of the names of forty-two phyla of prokaryotes. *International Journal of Systematic and Evolutionary Microbiology*, 71(10), 005056. <https://doi.org/10.1099/ijsem.0.005056>
- Orsi, W. D., Smith, J. M., Wilcox, H. M., Swallow, J. E., Carini, P., Worden, A. Z., & Santoro, A. E. (2015). Ecophysiology of uncultivated marine euryarchaea is linked to particulate organic matter. *The ISME Journal*, 9(8), 1747–1763. <https://doi.org/10.1038/ismej.2014.260>
- Pan, A., Yang, Q., Zhou, H., Ji, F., Wang, H., & Pancost, R. D. (2016). A diagnostic GDGT signature for the impact of hydrothermal activity on surface deposits at the Southwest Indian Ridge. *Organic Geochemistry*, 99, 90–101. <https://doi.org/10.1016/j.orggeochem.2016.07.001>
- Pancost, R. D., Coleman, J. M., Love, G. D., Chatzi, A., Bouloubassi, I., & Snape, C. E. (2008). Kerogen-bound glycerol dialkyl tetraether lipids released by hydropyrolysis of marine sediments: A bias against incorporation of sedimentary organisms? *Organic Geochemistry*, 39(9), 1359–1371. <https://doi.org/10.1016/j.orggeochem.2008.05.002>
- Pancost, R. D., Hopmans, E. C., & Sinninghe Damsté, J. S. (2001). Archaeal lipids in Mediterranean cold seeps: Molecular proxies for anaerobic methane oxidation. *Geochimica et Cosmochimica Acta*, 65(10), 1611–1627. [https://doi.org/10.1016/s0016-7037\(00\)00562-7](https://doi.org/10.1016/s0016-7037(00)00562-7)
- Pancost, R. D., & Sinninghe Damsté, J. S. (2003). Carbon isotopic compositions of prokaryotic lipids as tracers of carbon cycling in diverse settings. *Chemical Geology*, 195(1–4), 29–58. [https://doi.org/10.1016/s0009-2541\(02\)00387-x](https://doi.org/10.1016/s0009-2541(02)00387-x)
- Pancost, R. D., Sinninghe Damsté, J. S., de Lint, S., van der Maarel, M. J. E. C., & Gottschal, J. C., & The Medinut Shipboard Scientific Party. (2000). Biomarker Evidence for Widespread Anaerobic Methane Oxidation in Mediterranean Sediments by a Consortium of Methanogenic Archaea and Bacteria. *Applied and Environmental Microbiology*, 66(3), 1126–1132. <https://doi.org/10.1128/aem.66.3.1126-1132.2000>
- Parada, A. E., & Fuhrman, J. A. (2017). Marine archaeal dynamics and interactions with the microbial community over 5 years from surface to seafloor. *The ISME Journal*, 11(11), 2510–2525. <https://doi.org/10.1038/ismej.2017.104>
- Park, E., Hefter, J., Fischer, G., Iversen, M. H., Ramondenc, S., Nöthig, E.-M., & Mollenhauer, G. (2019). Seasonality of archaeal lipid flux and GDGT-based thermometry in sinking particles of high-latitude oceans: Fram Strait (79° N) and Antarctic Polar Front (50° S). *Biogeosciences*, 16(11), 2247–2268. <https://doi.org/10.5194/bg-16-2247-2019>
- Park, E., Hefter, J., Fischer, G., & Mollenhauer, G. (2018). TEX₈₆ in sinking particles in three eastern Atlantic upwelling regimes. *Organic Geochemistry*, 124, 151–163. <https://doi.org/10.1016/j.orggeochem.2018.07.015>
- Parks, D. H., Chuvpochina, M., Rinke, C., Mussig, A. J., Chaumeil, P.-A., & Hugenholtz, P. (2022). GTDB: An ongoing census of bacterial and archaeal diversity through a phylogenetically consistent, rank normalized and complete genome-based taxonomy. *Nucleic Acids Research*, 50(D1), D785–D794. <https://doi.org/10.1093/nar/gkab776>
- Pearson, A., Huang, Z., Ingalls, A. E., Romanek, C. S., Wiegand, J., Freeman, K. H., et al. (2004). Nonmarine Crenarchaeol in Nevada Hot Springs. *Applied and Environmental Microbiology*, 70(9), 5229–5237. <https://doi.org/10.1128/aem.70.9.5229-5237.2004>
- Pearson, A., Hurley, S. J., Elling, F. J., & Wilkes, E. B. (2019). CO₂-dependent carbon isotope fractionation in Archaea, Part I: Modeling the 3HP/4HB pathway. *Geochimica et Cosmochimica Acta*, 261, 368–382. <https://doi.org/10.1016/j.gca.2019.06.042>
- Pearson, A., Hurley, S. J., Walter, S. R. S., Kusch, S., Lichtin, S., & Zhang, Y. G. (2016). Stable carbon isotope ratios of intact GDGTs indicate heterogeneous sources to marine sediments. *Geochimica et Cosmochimica Acta*, 181, 18–35. <https://doi.org/10.1016/j.gca.2016.02.034>
- Pearson, A., McNichol, A. P., Benitez-Nelson, B. C., Hayes, J. M., & Eglinton, T. I. (2001). Origins of lipid biomarkers in Santa Monica Basin surface sediment: A case study using compound-specific $\delta^{14}\text{C}$ analysis. *Geochimica et Cosmochimica Acta*, 65(18), 3123–3137. [https://doi.org/10.1016/s0016-7037\(01\)00657-3](https://doi.org/10.1016/s0016-7037(01)00657-3)
- Pearson, P. N., van Dongen, B. E., Nicholas, C. J., Pancost, R. D., Schouten, S., Singano, J. M., & Wade, B. S. (2007). Stable warm tropical climate through the Eocene Epoch. *Geology*, 35(3), 211–214. <https://doi.org/10.1130/G23175A.1>

- Peterse, F., Kim, J.-H., Schouten, S., Kristensen, D. K., Koç, N., & Sinninghe Damsté, J. S. (2009). Constraints on the application of the MBT/CBT palaeothermometer at high latitude environments (Svalbard, Norway). *Organic Geochemistry*, 40(6), 692–699. <https://doi.org/10.1016/j.orggeochem.2009.03.004>
- Petrack, B., Reuning, L., Auer, G., Zhang, Y., Pfeiffer, M., & Schwark, L. (2023). Warm, not cold temperatures contributed to a Late Miocene reef decline in the Coral Sea. *Scientific Reports*, 13(1), 4015. <https://doi.org/10.1038/s41598-023-31034-8>
- Pitcher, A., Hopmans, E. C., Mosier, A. C., Park, S.-J., Rhee, S.-K., Francis, C. A., et al. (2011a). Core and intact polar glycerol dibiphytanyl glycerol tetraether lipids of ammonia-oxidizing archaea enriched from marine and estuarine sediments. *Applied and Environmental Microbiology*, 77(10), 3468–3477. <https://doi.org/10.1128/aem.02758-10>
- Pitcher, A., Villanueva, L., Hopmans, E. C., Schouten, S., Reichart, G.-J., & Sinninghe Damsté, J. S. (2011c). Niche segregation of ammonia-oxidizing archaea and anammox bacteria in the Arabian Sea oxygen minimum zone. *The ISME Journal*, 5(12), 1896–1904. <https://doi.org/10.1038/ismej.2011.60>
- Pitcher, A., Wuchter, C., Siedenberg, K., Schouten, S., & Sinninghe Damsté, J. S. (2011b). Crenarchaeol tracks winter blooms of ammonia-oxidizing Thaumarchaeota in the coastal North Sea. *Limnology and Oceanography*, 56(6), 2308–2318. <https://doi.org/10.4319/lo.2011.56.6.2308>
- Podlaska, A., Wakeham, S. G., Fanning, K. A., & Taylor, G. T. (2012). Microbial community structure and productivity in the oxygen minimum zone of the eastern tropical North Pacific. *Deep Sea Research Part I: Oceanographic Research Papers*, 66, 77–89. <https://doi.org/10.1016/j.dsr.2012.04.002>
- Polik, C. A., Eling, F. J., & Pearson, A. (2018). Impacts of Paleoecology on the TEX₈₆ Sea Surface Temperature Proxy in the Pliocene-Pleistocene Mediterranean Sea. *Paleoceanography and Paleoclimatology*, 33(12), 1472–1489. <https://doi.org/10.1029/2018pa003494>
- Prahl, F. G., Muehlhausen, L. A., & Zahnle, D. L. (1988). Further evaluation of long-chain alkenones as indicators of paleoceanographic conditions. *Geochimica et Cosmochimica Acta*, 52(9), 2303–2310. [https://doi.org/10.1016/0016-7037\(88\)90132-9](https://doi.org/10.1016/0016-7037(88)90132-9)
- Qian, P.-Y., Wang, Y., Lee, O. O., Lau, S. C. K., Yang, J., Lafi, F. F., et al. (2011). Vertical stratification of microbial communities in the Red Sea revealed by 16S rDNA pyrosequencing. *The ISME Journal*, 5(3), 507–518. <https://doi.org/10.1038/ismej.2010.112>
- Qin, W., Carlson, L. T., Armbrust, E. V., Devol, A. H., Moffett, J. W., Stahl, D. A., & Ingalls, A. E. (2015). Confounding effects of oxygen and temperature on the TEX₈₆ signature of marine Thaumarchaeota. *Proceedings of the National Academy of Sciences*, 112(35), 10979–10984. <https://doi.org/10.1073/pnas.1501568112>
- Qin, W., Heal, K. R., Ramdasi, R., Kobelt, J. N., Martens-Habben, W., Bertagnolli, A. D., et al. (2017). *Nitrosopumilus maritimus* gen. nov., sp. nov., *Nitrosopumilus cobalaminigenes* sp. nov., *Nitrosopumilus oxycloinae* sp. nov., and *Nitrosopumilus ureiphilus* sp. nov., four marine ammonia-oxidizing archaea of the phylum Thaumarchaeota. *International Journal of Systematic and Evolutionary Microbiology*, 67(12), 5067–5079. <https://doi.org/10.1099/ijsem.0.002416>
- Quehenberger, J., Pittenauer, E., Allmaier, G., & Spadiut, O. (2020). The influence of the specific growth rate on the lipid composition of *Sulfolobus acidocaldarius*. *Extremophiles*, 24(3), 413–420. <https://doi.org/10.1007/s00792-020-01165-1>
- Rattanasriampaipong, R., Tierney, J. E., Abell, J. T., & Gilmore, L. D. (2025). A Nutrient Effect on the TEX₈₆ Paleotemperature Proxy. *Geophysical Research Letters*, 52(12), e2025GL115237. <https://doi.org/10.1029/2025GL115237>
- Rattanasriampaipong, R., Zhang, Y. G., Pearson, A., Hedlund, B. P., & Zhang, S. (2022). Archaeal lipids trace ecology and evolution of marine ammonia-oxidizing archaea. *Proceedings of the National Academy of Sciences*, 119(31), e2123193119. <https://doi.org/10.1073/pnas.2123193119>
- Reeburgh, W. S. (1982). A major sink and flux control for methane in marine sediments; Anaerobic consumption. Retrieved from <https://pubs.usgs.gov/publication/70195654>
- Rempfert, K. R., Kraus, E. A., Nothaft, D. B., Dildar, N., Spear, J. R., Sepúlveda, J., & Templeton, A. S. (2023). Intact polar lipidome and membrane adaptations of microbial communities inhabiting serpentinite-hosted fluids. *Frontiers in Microbiology*, 14, 1198786. <https://doi.org/10.3389/fmicb.2023.1198786>
- Rhim, J. H., Kopf, S., McFarlin, J., Maloney, A. E., Batther, H., Harris, C. M., et al. (2024). Metabolic imprints in the hydrogen isotopes of *Archaeoglobus fulgidus* tetraether lipids. *Geochimica et Cosmochimica Acta*, 386, 196–212. <https://doi.org/10.1016/j.gca.2024.09.032>
- Rice, A., Nooteboom, P. D., van Sebille, E., Peterse, F., Ziegler, M., & Sluijs, A. (2022). Limited lateral transport bias during export of sea surface temperature proxy carriers in the Mediterranean Sea. *Geophysical Research Letters*, 49(4), e2021GL096859. <https://doi.org/10.1029/2021GL096859>
- Rice, A., Park, E., Mollenhauer, G., Bouwmans, D., van Bostel, A., de Lange, G. J., et al. (2026). Seasonal changes in marine archaeal tetraether lipid export depth linked to net primary productivity. *Paleoceanography and Paleoclimatology*, 41(2), e2025PA005141. <https://doi.org/10.1029/2025PA005141>
- Richey, J. N., & Tierney, J. E. (2016). GDGT and alkenone flux in the northern Gulf of Mexico: Implications for the TEX₈₆ and UK'37 paleothermometers. *Paleoceanography*, 31(12), 1547–1561. <https://doi.org/10.1002/2016PA003032>
- Rinke, C., Chuvochina, M., Mussig, A. J., Chaumeil, P.-A., Davin, A. A., Waite, D. W., et al. (2021). A standardized archaeal taxonomy for the Genome Taxonomy Database. *Nature Microbiology*, 6(7), 946–959. <https://doi.org/10.1038/s41564-021-00918-8>
- Rinke, C., Rubino, F., Messer, L. F., Youssef, N., Parks, D. H., Chuvochina, M., et al. (2019). A phylogenomic and ecological analysis of the globally abundant Marine Group II archaea (*Ca. Poseidoniales* ord. nov.). *The ISME Journal*, 13(13), 663–675. <https://doi.org/10.1038/s41396-018-0282-y>
- Robinson, S. A., Ruhl, M., Astley, D. L., Naafs, B. D. A., Farnsworth, A. J., Bown, P. R., et al. (2017). Early Jurassic North Atlantic sea-surface temperatures from TEX₈₆ palaeothermometry. *Sedimentology*, 64(1), 215–230. <https://doi.org/10.1111/sed.12321>
- Rodrigo-Gámiz, M., Rampen, S. W., de Haas, H., Baas, M., Schouten, S., & Sinninghe Damsté, J. S. (2015). Constraints on the applicability of the organic temperature proxies U₃₇^K, TEX₈₆ and LDI in the subpolar region around Iceland. *Biogeosciences*, 12(22), 6573–6590. <https://doi.org/10.5194/bg-12-6573-2015>
- Rommerskirchen, F., Condon, T., Mollenhauer, G., Dupont, L., & Schefuss, E. (2011). Miocene to Pliocene development of surface and subsurface temperatures in the Benguela Current system. *Paleoceanography*, 26(3), PA3216. <https://doi.org/10.1029/2010pa002074>
- Rossel, P. E., Elvert, M., Ramette, A., Boetius, A., & Hinrichs, K.-U. (2011). Factors controlling the distribution of anaerobic methanotrophic communities in marine environments: Evidence from intact polar membrane lipids. *Geochimica et Cosmochimica Acta*, 75(1), 164–184. <https://doi.org/10.1016/j.gca.2010.09.031>
- Rossel, P. E., Lipp, J. S., Fredricks, H. F., Arnds, J., Boetius, A., Elvert, M., & Hinrichs, K.-U. (2008). Intact polar lipids of anaerobic methanotrophic archaea and associated bacteria. *Organic Geochemistry*, 39(8), 992–999. <https://doi.org/10.1016/j.orggeochem.2008.02.021>
- Rowland, S. J. (1990). Production of acyclic isoprenoid hydrocarbons by laboratory maturation of methanogenic bacteria. *Organic Geochemistry*, 15(1), 9–16. [https://doi.org/10.1016/0146-6380\(90\)90181-X](https://doi.org/10.1016/0146-6380(90)90181-X)

- Sabino, M., Birgel, D., Natalicchio, M., Dela Pierre, F., & Peckmann, J. (2022). Carbon isotope excursions during the late Miocene recorded by lipids of marine Thaumarchaeota, Piedmont Basin, Mediterranean Sea. *Geology*, 50(1), 32–36. <https://doi.org/10.1130/g49360.1>
- Sangiorgi, F., Bijl, P. K., Passchier, S., Salzmann, U., Schouten, S., McKay, R., et al. (2018). Southern Ocean warming and Wilkes Land ice sheet retreat during the mid-Miocene. *Nature Communications*, 9(1), 317. <https://doi.org/10.1038/s41467-017-02609-7>
- Santoro, A. E., Bayer, B., Elling, F. J., & Pearson, A. (2021). *Candidatus Nitrosopelagicus*. In *Bergey's Manual of Systematics of Archaea and Bacteria* (pp. 1–13). American Cancer Society. <https://doi.org/10.1002/9781118960608.gbm01969>
- Santoro, A. E., Casciotti, K. L., & Francis, C. A. (2010). Activity, abundance and diversity of nitrifying archaea and bacteria in the central California Current. *Environmental Microbiology*, 12(7), 1989–2006. <https://doi.org/10.1111/j.1462-2920.2010.02205.x>
- Santoro, A. E., Richter, R. A., & Dupont, C. L. (2019). Planktonic Marine Archaea. *Annual Review of Marine Science*, 11(1), 131–158. <https://doi.org/10.1146/annurev-marine-121916-063141>
- Santoro, A. E., Saito, M. A., Goepfert, T. J., Lamborg, C. H., Dupont, C. L., & DiTullio, G. R. (2017). Thaumarchaeal ecotype distributions across the equatorial Pacific Ocean and their potential roles in nitrification and sinking flux attenuation. *Limnology and Oceanography*, 62(5), 1984–2003. <https://doi.org/10.1002/lno.10547>
- Santos, M., Bröder, L., O'Regan, M., Hernández-Almeida, I., Tesi, T., Bigler, L., et al. (2026). Holocene sea ice and paleoenvironment conditions in the Beaufort Sea (Canadian Arctic) reconstructed with lipid biomarkers. *Climate of the Past*, 22(1), 187–203. <https://doi.org/10.5194/cp-22-187-2026>
- Schattenhofer, M., Fuchs, B. M., Amann, R., Zubkov, M. V., Tarran, G. A., & Pernthaler, J. (2009). Latitudinal distribution of prokaryotic picoplankton populations in the Atlantic Ocean. *Environmental Microbiology*, 11(8), 2078–2093. <https://doi.org/10.1111/j.1462-2920.2009.01929.x>
- Schattenhofer, M., Wulf, J., Kostadinov, I., Glöckner, F. O., Zubkov, M. V., & Fuchs, B. M. (2011). Phylogenetic characterisation of picoplanktonic populations with high and low nucleic acid content in the North Atlantic Ocean. *Systematic and Applied Microbiology*, 34(6), 470–475. <https://doi.org/10.1016/j.syapm.2011.01.008>
- Schleper, C., Jurgens, G., & Jonuscheit, M. (2005). Genomic studies of uncultivated archaea. *Nature Reviews Microbiology*, 3(6), 479–488. <https://doi.org/10.1038/nrmicro1159>
- Schmidt, F., Hinrichs, K.-U., & Elvert, M. (2010). Sources, transport, and partitioning of organic matter at a highly dynamic continental margin. *Marine Chemistry*, 118(1–2), 37–55. <https://doi.org/10.1016/j.marchem.2009.10.003>
- Schoon, P. L., Heilmann-Clausen, C., Pagh Schultz, B., Sluijs, A., Sinninghe Damsté, J. S., & Schouten, S. (2013). Recognition of Early Eocene global carbon isotope excursions using lipids of marine Thaumarchaeota. *Earth and Planetary Science Letters*, 373, 160–168. <https://doi.org/10.1016/j.epsl.2013.04.037>
- Schouten, S., Baas, M., Hopmans, E. C., & Sinninghe Damsté, J. S. (2008a). An unusual isoprenoid tetraether lipid in marine and lacustrine sediments. *Organic Geochemistry*, 39(8), 1033–1038. <https://doi.org/10.1016/j.orggeochem.2008.01.019>
- Schouten, S., Forster, A., Panoto, F. E., & Sinninghe Damsté, J. S. (2007b). Towards calibration of the TEX₈₆ palaeothermometer for tropical sea surface temperatures in ancient greenhouse worlds. *Organic Geochemistry*, 38(9), 1537–1546. <https://doi.org/10.1016/j.orggeochem.2007.05.014>
- Schouten, S., Hoefs, M. J. L., Koopmans, M. P., Bosch, H.-J., & Sinninghe Damsté, J. S. (1998). Structural characterization, occurrence and fate of archaeal ether-bound acyclic and cyclic biphytanes and corresponding diols in sediments. *Organic Geochemistry*, 29(5–7), 1305–1319. [https://doi.org/10.1016/S0146-6380\(98\)00131-4](https://doi.org/10.1016/S0146-6380(98)00131-4)
- Schouten, S., Hopmans, E. C., Baas, M., Boumann, H., Standfest, S., Könneke, M., et al. (2008b). Intact membrane lipids of “*Candidatus Nitrosopumilus maritimus*,” a cultivated representative of the cosmopolitan mesophilic group I crenarchaeota. *Applied and Environmental Microbiology*, 74(8), 2433–2440. <https://doi.org/10.1128/AEM.01709-07>
- Schouten, S., Hopmans, E. C., Forster, A., van Breugel, Y., Kuypers, M. M. M., & Sinninghe Damsté, J. S. (2003b). Extremely high sea-surface temperatures at low latitudes during the middle Cretaceous as revealed by archaeal membrane lipids. *Geology*, 31(12), 1069–1072. <https://doi.org/10.1130/g19876.1>
- Schouten, S., Hopmans, E. C., Pancost, R. D., & Sinninghe Damsté, J. S. (2000). Widespread occurrence of structurally diverse tetraether membrane lipids: Evidence for the ubiquitous presence of low-temperature relatives of hyperthermophiles. *Proceedings of the National Academy of Sciences*, 97(26), 14421–14426. <https://doi.org/10.1073/pnas.97.26.14421>
- Schouten, S., Hopmans, E. C., Rosell-Melé, A., Pearson, A., Adam, P., Bauersachs, T., et al. (2013a). An interlaboratory study of TEX₈₆ and BIT analysis of sediments, extracts, and standard mixtures: TEX₈₆ and BIT Index Round Robin. *Geochemistry, Geophysics, Geosystems*, 14(12), 5263–5285. <https://doi.org/10.1002/2013gc004904>
- Schouten, S., Hopmans, E. C., Schefuß, E., & Sinninghe Damsté, J. S. (2002). Distributional variations in marine crenarchaeotal membrane lipids: A new tool for reconstructing ancient sea water temperatures? *Earth and Planetary Science Letters*, 204(1–2), 265–274. [https://doi.org/10.1016/S0012-821X\(02\)00979-2](https://doi.org/10.1016/S0012-821X(02)00979-2)
- Schouten, S., Hopmans, E. C., & Sinninghe Damsté, J. S. (2004). The effect of maturity and depositional redox conditions on archaeal tetraether lipid palaeothermometry. *Organic Geochemistry*, 35(5), 567–571. <https://doi.org/10.1016/j.orggeochem.2004.01.012>
- Schouten, S., Hopmans, E. C., & Sinninghe Damsté, J. S. (2013b). The organic geochemistry of glycerol dialkyl glycerol tetraether lipids: A review. *Organic Geochemistry*, 54, 19–61. <https://doi.org/10.1016/j.orggeochem.2012.09.006>
- Schouten, S., Hugué, C., Hopmans, E. C., Kienhuis, M. V. M., & Sinninghe Damsté, J. S. (2007a). Analytical methodology for TEX₈₆ Palaeothermometry by high-performance liquid chromatography/atmospheric pressure chemical ionization-mass spectrometry. *Analytical Chemistry*, 79(7), 2940–2944. <https://doi.org/10.1021/ac062339v>
- Schouten, S., Middelburg, J. J., Hopmans, E. C., & Sinninghe Damsté, J. S. (2010). Fossilization and degradation of intact polar lipids in deep subsurface sediments: A theoretical approach. *Geochimica et Cosmochimica Acta*, 74(13), 3806–3814. <https://doi.org/10.1016/j.gca.2010.03.029>
- Schouten, S., Pitcher, A., Hopmans, E. C., Villanueva, L., van Bleijswijk, J., & Sinninghe Damsté, J. S. (2012). Intact polar and core glycerol dibiphytanyl glycerol tetraether lipids in the Arabian Sea oxygen minimum zone: I. Selective preservation and degradation in the water column and consequences for the TEX₈₆. *Geochimica et Cosmochimica Acta*, 98, 228–243. <https://doi.org/10.1016/j.gca.2012.05.002>
- Schouten, S., Villanueva, L., Hopmans, E. C., van der Meer, M. T. J., & Sinninghe Damsté, J. S. (2014). Are Marine Group II Euryarchaeota significant contributors to tetraether lipids in the ocean? *Proceedings of the National Academy of Sciences*, 111(41), E4285. <https://doi.org/10.1073/pnas.1416176111>
- Schouten, S., Wakeham, S. G., Hopmans, E. C., & Sinninghe Damsté, J. S. (2003a). Biogeochemical Evidence that Thermophilic Archaea Mediate the Anaerobic Oxidation of Methane. *Applied and Environmental Microbiology*, 69(3), 1680–1686. <https://doi.org/10.1128/aem.69.3.1680-1686.2003>

- Schouten, S., Wakeham, S. G., & Sinninghe Damsté, J. S. (2001). Evidence for anaerobic methane oxidation by archaea in euxinic waters of the Black Sea. *Organic Geochemistry*, 32(10), 1277–1281. [https://doi.org/10.1016/S0146-6380\(01\)00110-3](https://doi.org/10.1016/S0146-6380(01)00110-3)
- Schubert, C. J., Coolen, M. J. L., Neretin, L. N., Schippers, A., Abbas, B., Durisch-Kaiser, E., et al. (2006). Aerobic and anaerobic methanotrophs in the Black Sea water column. *Environmental Microbiology*, 8(10), 1844–1856. <https://doi.org/10.1111/j.1462-2920.2006.01079.x>
- Schubotz, F., Lipp, J. S., Elvert, M., & Hinrichs, K.-U. (2011). Stable carbon isotopic compositions of intact polar lipids reveal complex carbon flow patterns among hydrocarbon degrading microbial communities at the Chapopote asphalt volcano. *Geochimica et Cosmochimica Acta*, 75(16), 4399–4415. <https://doi.org/10.1016/j.gca.2011.05.018>
- Schubotz, F., Wakeham, S. G., Lipp, J. S., Fredricks, H. F., & Hinrichs, K.-U. (2009). Detection of microbial biomass by intact polar membrane lipid analysis in the water column and surface sediments of the Black Sea. *Environmental Microbiology*, 11(10), 2720–2734. <https://doi.org/10.1111/j.1462-2920.2009.01999.x>
- Schukies, J. (2018). Concentrations of glycerol dialkyl glycerol tetraethers (GDGTs) in core top sediments from continental slope off Newfoundland, Orphan Knoll Region. *PANGAEA*. <https://doi.org/10.1594/PANGAEA.894305>
- Sehgal, S. N., Kates, M., & Gibbons, N. E. (1962). Lipids of *Halobacterium cutirubrum*. *Canadian Journal of Biochemistry and Physiology*, 40(1), 69–81. <https://doi.org/10.1139/y62-011>
- Seki, O., Bendle, J. A., Harada, N., Kobayashi, M., Sawada, K., Moossen, H., et al. (2014). Assessment and calibration of TEX₈₆ paleothermometry in the Sea of Okhotsk and sub-polar North Pacific region: Implications for paleoceanography. *Progress in Oceanography*, 126, 254–266. <https://doi.org/10.1016/j.poc.2014.04.013>
- Shah, S. R., Mollenhauer, G., Ohkouchi, N., Eglinton, T. I., & Pearson, A. (2008). Origins of archaeal tetraether lipids in sediments: Insights from radiocarbon analysis. *Geochimica et Cosmochimica Acta*, 72(18), 4577–4594. <https://doi.org/10.1016/j.gca.2008.06.021>
- Shimada, H., Nemoto, N., Shida, Y., Oshima, T., & Yamagishi, A. (2002). Complete polar lipid composition of *Thermoplasma acidophilum* HO-62 determined by high-performance liquid chromatography with evaporative light-scattering detection. *Journal of Bacteriology*, 184(2), 556–563. <https://doi.org/10.1128/jb.184.2.556-563.2002>
- Sinninghe Damsté, J. S. (2016). Spatial heterogeneity of sources of branched tetraethers in shelf systems: The geochemistry of tetraethers in the Berau River delta (Kalimantan, Indonesia). *Geochimica et Cosmochimica Acta*, 186, 13–31. <https://doi.org/10.1016/j.gca.2016.04.033>
- Sinninghe Damsté, J. S., Ossebaard, J., Schouten, S., & Verschuren, D. (2012a). Distribution of tetraether lipids in the 25-ka sedimentary record of Lake Challa: Extracting reliable TEX₈₆ and MBT/CBT palaeotemperatures from an equatorial African lake. *Quaternary Science Reviews*, 50, 43–54. <https://doi.org/10.1016/j.quascirev.2012.07.001>
- Sinninghe Damsté, J. S., Rijpstra, W. I. C., Hopmans, E. C., den Uijl, M. J., Weijers, J. W. H., & Schouten, S. (2018). The enigmatic structure of the crenarchaeol isomer. *Organic Geochemistry*, 124, 22–28. <https://doi.org/10.1016/j.orggeochem.2018.06.005>
- Sinninghe Damsté, J. S., Rijpstra, W. I. C., Hopmans, E. C., Jung, M.-Y., Kim, J.-G., Rhee, S.-K., et al. (2012b). Intact polar and core glycerol dibiphytanyl glycerol tetraether lipids of group I.1a and I.1b Thaumarchaeota in soil. *Applied and Environmental Microbiology*, 78(19), 6866–6874. <https://doi.org/10.1128/aem.01681-12>
- Sinninghe Damsté, J. S., Rijpstra, W. I. C., Hopmans, E. C., Weijers, J. W. H., Foessel, B. U., Overmann, J., & Dedysh, S. N. (2011). 13,16-dimethyl octacosanedioic acid (*iso*-Diabolic Acid), a common membrane-spanning lipid of acidobacteria subdivisions 1 and 3. *Applied and Environmental Microbiology*, 77(12), 4147–4154. <https://doi.org/10.1128/aem.00466-11>
- Sinninghe Damsté, J. S., Schouten, S., Hopmans, E. C., van Duin, A. C. T., & Geenevasen, J. A. J. (2002). Crenarchaeol: The characteristic core glycerol dibiphytanyl glycerol tetraether membrane lipid of cosmopolitan pelagic crenarchaeota. *Journal of Lipid Research*, 43(10), 1641–1651.
- Sinninghe Damsté, J. S., Warden, L. A., Berg, C., Jürgens, K., & Moros, M. (2022). Evaluation of the distributions of hydroxylated glycerol dibiphytanyl glycerol tetraethers (GDGTs) in Holocene Baltic Sea sediments for reconstruction of sea surface temperature: The effect of changing salinity. *Climate of the Past*, 18(10), 2271–2288. <https://doi.org/10.5194/cp-18-2271-2022>
- Sintes, E., Bergauer, K., De Corte, D., Yokokawa, T., & Herndl, G. J. (2013). Archaeal *amo* A gene diversity points to distinct biogeography of ammonia-oxidizing *Crenarchaeota* in the ocean. *Environmental Microbiology*, 15(5), 1647–1658. <https://doi.org/10.1111/j.1462-2920.2012.02801.x>
- Sintes, E., De Corte, D., Haberleitner, E., & Herndl, G. J. (2016). Geographic Distribution of Archaeal Ammonia Oxidizing Ecotypes in the Atlantic Ocean. *Frontiers in Microbiology*, 7, 77. <https://doi.org/10.3389/fmicb.2016.00077>
- Śliwińska, K. K., Coxall, H. K., Hutchinson, D. K., Liebrand, D., Schouten, S., & de Boer, A. M. (2023). Sea surface temperature evolution of the North Atlantic Ocean across the Eocene–Oligocene transition. *Climate of the Past*, 19(1), 123–140. <https://doi.org/10.5194/cp-19-123-2023>
- Sluijs, A., Frieling, J., Inglis, G. N., Nierop, K. G. J., Peterse, F., Sangiorgi, F., & Schouten, S. (2020). Late Paleocene–early Eocene Arctic Ocean sea surface temperatures: Reassessing biomarker paleothermometry at Lomonosov Ridge. *Climate of the Past*, 16(6), 2381–2400. <https://doi.org/10.5194/cp-16-2381-2020>
- Sluijs, A., Schouten, S., Pagani, M., Wolterring, M., Brinkhuis, H., Sinninghe Damsté, J. S., et al. (2006). Subtropical Arctic Ocean temperatures during the Palaeocene/Eocene thermal maximum. *Nature*, 441(7093), 610–613. <https://doi.org/10.1038/nature04668>
- Smittenberg, R. H., Hopmans, E. C., Schouten, S., Hayes, J. M., Eglinton, T. I., & Sinninghe Damsté, J. S. (2004). Compound-specific radiocarbon dating of the varved Holocene sedimentary record of Saanich Inlet, Canada. *Paleoceanography*, 19(2), PA2012. <https://doi.org/10.1029/2003PA000927>
- Sollai, M., Villanueva, L., Hopmans, E. C., Keil, R. G., & Sinninghe Damsté, J. S. (2019b). Archaeal sources of intact membrane lipid biomarkers in the oxygen deficient zone of the eastern tropical South Pacific. *Frontiers in Microbiology*, 10, 765. <https://doi.org/10.3389/fmicb.2019.00765>
- Sollai, M., Villanueva, L., Hopmans, E. C., Reichart, G.-J., & Sinninghe Damsté, J. S. (2019a). A combined lipidomic and 16S rRNA gene amplicon sequencing approach reveals archaeal sources of intact polar lipids in the stratified Black Sea water column. *Geobiology*, 17(1), 91–109. <https://doi.org/10.1111/gbi.12316>
- Sollich, M., Yoshinaga, M. Y., Häusler, S., Price, R. E., Hinrichs, K.-U., & Bühring, S. I. (2017). Heat stress dictates microbial lipid composition along a thermal gradient in marine sediments. *Frontiers in Microbiology*, 8, 1550. <https://doi.org/10.3389/fmicb.2017.01550>
- Spang, A., Caceres, E. F., & Ettema, T. J. G. (2017). Genomic exploration of the diversity, ecology, and evolution of the archaeal domain of life. *Science*, 357(6351), eaaf3883. <https://doi.org/10.1126/science.aaf3883>
- Sparkes, R. B., Doğrul Selver, A., Bischoff, J., Talbot, H. M., Gustafsson, Ö., Semiletov, I. P., et al. (2015). GDGT distributions on the East Siberian Arctic Shelf: Implications for organic carbon export, burial and degradation. *Biogeosciences*, 12(12), 3753–3768. <https://doi.org/10.5194/bg-12-3753-2015>
- Spencer-Jones, C. L., McClymont, E. L., Bale, N. J., Hopmans, E. C., Schouten, S., Müller, J., et al. (2021). Archaeal intact polar lipids in polar waters: A comparison between the Amundsen and Scotia seas. *Biogeosciences*, 18(11), 3485–3504. <https://doi.org/10.5194/bg-18-3485-2021>

- Stadnitskaia, A., Baas, M., Ivanov, M. K., Van Weering, T. C. E., & Sinninghe Damsté, J. S. (2003). Novel archaeal macrocyclic diether core membrane lipids in a methane-derived carbonate crust from a mud volcano in the Sorokin Trough, NE Black Sea. *Archaea*, 1(3), 165–173. <https://doi.org/10.1155/2003/329175>
- Stadnitskaia, A., Bouloubassi, I., Elvert, M., Hinrichs, K.-U., & Sinninghe Damsté, J. S. (2008). Extended hydroxyarchaeol, a novel lipid biomarker for anaerobic methanotrophy in cold seepage habitats. *Organic Geochemistry*, 39(8), 1007–1014. <https://doi.org/10.1016/j.orggeochem.2008.04.019>
- Stahl, D. A., & de la Torre, J. R. (2012). Physiology and diversity of ammonia-oxidizing Archaea. *Annual Review of Microbiology*, 66(1), 83–101. <https://doi.org/10.1146/annurev-micro-092611-150128>
- Stieglmeier, M., Klingl, A., Alves, R. J. E., Rittmann, S. K.-M. R., Melcher, M., Leisch, N., & Schleper, C. (2014). *Nitrososphaera viennensis* gen. nov., sp. nov., an aerobic and mesophilic, ammonia-oxidizing archaeon from soil and a member of the archaeal phylum Thaumarchaeota. *International Journal of Systematic and Evolutionary Microbiology*, 64(Pt 8), 2738–2752. <https://doi.org/10.1099/ijs.0.063172-0>
- Sturt, H. F., Summons, R. E., Smith, K., Elvert, M., & Hinrichs, K.-U. (2004). Intact polar membrane lipids in prokaryotes and sediments deciphered by high-performance liquid chromatography/electrospray ionization multistage mass spectrometry—New biomarkers for biogeochemistry and microbial ecology. *Rapid Communications in Mass Spectrometry*, 18(6), 617–628. <https://doi.org/10.1002/rcm.1378>
- Suzuki, K., Yamamoto, M., Park, Y.-H., & Nam, S.-I. (2025). Stepwise cooling events in the western Arctic at 8.2 and 4.2 ka: Proxy Development and Application. *Paleoceanography and Paleoclimatology*, 40(12), e2025PA005239. <https://doi.org/10.1029/2025PA005239>
- Swain, M., Brisson, J.-R., Sprott, G. D., Cooper, F. P., & Patel, G. B. (1997). Identification of β -L-glucose as the sugar moiety of the main polar lipid *Thermoplasma acidophilum*. *Biochimica et Biophysica Acta*, 1345(1), 56–64. [https://doi.org/10.1016/S0005-2760\(96\)00163-4](https://doi.org/10.1016/S0005-2760(96)00163-4)
- Tachibana, A., Tanaka, T., Taniguchi, M., & Susumu, O. (1993). Purification and Characterization of Geranylgeranyl Diphosphate Synthase from *Methanobacterium thermoformicum* SF-4. *Bioscience, Biotechnology, and Biochemistry*, 57(7), 1129–1133. <https://doi.org/10.1271/bbb.57.1129>
- Tachibana, A., Yano, Y., Otani, S., Nomura, N., Sako, Y., & Taniguchi, M. (2000). Novel prenyltransferase gene encoding farnesylgeranyl diphosphate synthase from a hyperthermophilic archaeon, *Aeropyrum pernix*. *European Journal of Biochemistry*, 267(2), 321–328. <https://doi.org/10.1046/j.1432-1327.2000.00967.x>
- Takai, K., & Nakamura, K. (2011). Archaeal diversity and community development in deep-sea hydrothermal vents. *Current Opinion in Microbiology*, 14(3), 282–291. <https://doi.org/10.1016/j.mib.2011.04.013>
- Takano, Y., Chikaraishi, Y., Ogawa, N. O., Nomaki, H., Morono, Y., Inagaki, F., et al. (2010). Sedimentary membrane lipids recycled by deep-sea benthic archaea. *Nature Geoscience*, 3(12), 858–861. <https://doi.org/10.1038/ngeo983>
- Taylor, K. W. R., Huber, M., Hollis, C. J., Hernandez-Sanchez, M. T., & Pancost, R. D. (2013). Re-evaluating modern and Palaeogene GDGT distributions: Implications for SST reconstructions. *Global and Planetary Change*, 108, 158–174. <https://doi.org/10.1016/j.gloplacha.2013.06.011>
- Teira, E., Lebaron, P., van Aken, H., & Herndl, G. J. (2006). Distribution and activity of Bacteria and Archaea in the deep water masses of the North Atlantic. *Limnology and Oceanography*, 51(5), 2131–2144. <https://doi.org/10.4319/lo.2006.51.5.2131>
- Teske, A., & Sørensen, K. B. (2008). Uncultured archaea in deep marine subsurface sediments: Have we caught them all? *The ISME Journal*, 2(1), 3–18. <https://doi.org/10.1038/ismej.2007.90>
- The Cenozoic CO₂ Proxy Integration Project (CENCO2PIP) Consortium (2023). Toward a Cenozoic history of atmospheric CO₂. *Science*, 382(6675), eadi5177. <https://doi.org/10.1126/science.adi5177>
- Thiel, V., Toporski, J., Schumann, G., Sjövall, P., & Lausmaa, J. (2007). Analysis of archaeal core ether lipids using Time of Flight—Secondary Ion Mass Spectrometry (ToF-SIMS): Exploring a new prospect for the study of biomarkers in geobiology. *Geobiology*, 5(1), 75–83. <https://doi.org/10.1111/j.1472-4669.2006.00093.x>
- Thomas, E. K., Clemens, S. C., Prell, W. L., Herbert, T. D., Huang, Y., Liu, Z., et al. (2014). Temperature and leaf wax $\delta^2\text{H}$ records demonstrate seasonal and regional controls on Asian monsoon proxies. *Geology*, 42(12), 1075–1078. <https://doi.org/10.1130/G36289.1>
- Tierney, J. E., Sinninghe Damsté, J. S., Pancost, R. D., Sluijs, A., & Zachos, J. C. (2017). Eocene temperature gradients. *Nature Geoscience*, 10(8), 538–539. <https://doi.org/10.1038/ngeo2997>
- Tierney, J. E., & Tingley, M. P. (2014). A Bayesian, spatially-varying calibration model for the TEX₈₆ proxy. *Geochimica et Cosmochimica Acta*, 127, 83–106. <https://doi.org/10.1016/j.gca.2013.11.026>
- Tierney, J. E., & Tingley, M. P. (2015). A TEX₈₆ surface sediment database and extended Bayesian calibration. *Scientific Data*, 2(1), 150029. <https://doi.org/10.1038/sdata.2015.29>
- Tierney, J. E., & Tingley, M. P. (2018). BAYSPLINE: A New Calibration for the Alkenone Paleothermometer. *Paleoceanography and Paleoclimatology*, 33(3), 281–301. <https://doi.org/10.1002/2017pa003201>
- Tierney, J. E., Ummenhofer, C. C., & de Menocal, P. B. (2015). Past and future rainfall in the Horn of Africa. *Science Advances*, 1(9), e1500682. <https://doi.org/10.1126/sciadv.1500682>
- Tindall, B. J., Ross, H. N. M., & Grant, W. D. (1984). *Natronobacterium* gen. nov. and *Natronococcus* gen. nov., Two New Genera of Halophilic Archaeobacteria. *Systematic and Applied Microbiology*, 5(1), 41–57. [https://doi.org/10.1016/S0723-2020\(84\)80050-8](https://doi.org/10.1016/S0723-2020(84)80050-8)
- Tolar, B. B., Reji, L., Smith, J. M., Blum, M., Pennington, J. T., Chavez, F. P., & Francis, C. A. (2020). Time series assessment of Thaumarchaeota ecotypes in Monterey Bay reveals the importance of water column position in predicting distribution–environment relationships. *Limnology and Oceanography*, 65(9), 2041–2055. <https://doi.org/10.1002/lno.11436>
- Tourte, M., Schaeffer, P., Grossi, V., & Oger, P. M. (2022). Membrane adaptation in the hyperthermophilic archaeon *Pyrococcus furiosus* relies upon a novel strategy involving glycerol monoalkyl glycerol tetraether lipids. *Environmental Microbiology*, 24(4), 2029–2046. <https://doi.org/10.1111/1462-2920.15923>
- Trincone, A., Lanzotti, V., Nicolaus, B., Zillig, W., De Rosa, M., & Gambacorta, A. (1989). Comparative Lipid Composition of Aerobically and Anaerobically Grown *Desulfurolobus ambivalens*, an Autotrophic Thermophilic Archaeobacterium. *Journal of General Microbiology*, 135(10), 2751–2757. <https://doi.org/10.1099/00221287-135-10-2751>
- Trommer, G., Siccha, M., van der Meer, M. T. J., Schouten, S., Sinninghe Damsté, J. S., Schulz, H., et al. (2009). Distribution of Crenarchaeota tetraether membrane lipids in surface sediments from the Red Sea. *Organic Geochemistry*, 40(6), 724–731. <https://doi.org/10.1016/j.orggeochem.2009.03.001>
- Turich, C., Freeman, K. H., Bruns, M. A., Conte, M., Jones, A. D., & Wakeham, S. G. (2007). Lipids of marine Archaea: Patterns and provenance in the water-column and sediments. *Geochimica et Cosmochimica Acta*, 71(13), 3272–3291. <https://doi.org/10.1016/j.gca.2007.04.013>
- Turich, C., Schouten, S., Thunell, R. C., Varela, R., Astor, Y., & Wakeham, S. G. (2013). Comparison of TEX₈₆ and U₃₇ temperature proxies in sinking particles in the Cariaco Basin. *Deep Sea Research Part I: Oceanographic Research Papers*, 78, 115–133. <https://doi.org/10.1016/j.dsr.2013.02.008>

- Uda, I., Sugai, A., Itoh, Y. H., & Itoh, T. (2001). Variation in molecular species of polar lipids from *Thermoplasma acidophilum* depends on growth temperature. *Lipids*, 36(1), 103–105. <https://doi.org/10.1007/s11745-001-0914-2>
- Ulloa, O., Canfield, D. E., DeLong, E. F., Letelier, R. M., & Stewart, F. J. (2012). Microbial oceanography of anoxic oxygen minimum zones. *Proceedings of the National Academy of Sciences*, 109(40), 15996–16003. <https://doi.org/10.1073/pnas.1205009109>
- Umoh, U. U., Li, L., Luckge, A., Schwartz-Schampera, U., & Naafs, B. D. A. (2020). Influence of hydrothermal vent activity on GDGT pool in marine sediments might be less than previously thought. *Organic Geochemistry*, 149, 104102. <https://doi.org/10.1016/j.orggeochem.2020.104102>
- Umoh, U. U., Li, L., Wang, J., Kauluma, N., Asuquo, F. E., & Akpan, E. R. (2022). Glycerol dialkyl glycerol tetraether signatures in tropical mesotidal estuary sediments of Qua Iboe River, Gulf of Guinea. *Organic Geochemistry*, 170, 104461. <https://doi.org/10.1016/j.orggeochem.2022.104461>
- van der Meer, M. T. J., Baas, M., Rijpstra, W. I. C., Marino, G., Rohling, E. J., Sinninghe Damsté, J. S., & Schouten, S. (2007). Hydrogen isotopic compositions of long-chain alkenones record freshwater flooding of the Eastern Mediterranean at the onset of sapropel deposition. *Earth and Planetary Science Letters*, 262(3–4), 594–600. <https://doi.org/10.1016/j.epsl.2007.08.014>
- van der Weijst, C. M. H., van der Laan, K. J., Peterse, F., Reichart, G.-J., Sangiorgi, F., Schouten, S., et al. (2022). A 15-million-year surface- and subsurface-integrated TEX₈₆ temperature record from the eastern equatorial Atlantic. *Climate of the Past*, 18(8), 1947–1962. <https://doi.org/10.5194/cp-18-1947-2022>
- van Kemenade, Z. R., Kusch, S., Berg, S., Hopmans, E. C., Van Der Meer, M. T. J., & Rush, D. (2025). Bacterioplanepolyols and glycerol dialkyl glycerol tetraethers record Holocene redox regime shifts in a marine inlet in eastern Prydz Bay, Antarctica. *Organic Geochemistry*, 206, 105011. <https://doi.org/10.1016/j.orggeochem.2025.105011>
- Varma, D., Hättig, K., van der Meer, M. T. J., Reichart, G.-J., & Schouten, S. (2023). Constraining Water Depth Influence on Organic Paleo-temperature Proxies Using Sedimentary Archives. *Paleoceanography and Paleoclimatology*, 38(6), e2022PA004533. <https://doi.org/10.1029/2022PA004533>
- Varma, D., Hopmans, E. C., van Kemenade, Z. R., Kusch, S., Berg, S., Bale, N. J., et al. (2024b). Evaluating isoprenoidal hydroxylated GDGT-based temperature proxies in surface sediments from the global ocean. *Geochimica et Cosmochimica Acta*, 370, 113–127. <https://doi.org/10.1016/j.gca.2023.12.019>
- Varma, D., van der Meer, M. T. J., Reichart, G.-J., & Schouten, S. (2024c). Impact of water depth on the distributions and proxies of isoprenoidal hydroxylated GDGTs in the Mediterranean Sea and the Red Sea. *Organic Geochemistry*, 194, 104780. <https://doi.org/10.1016/j.orggeochem.2024.104780>
- Varma, D., Villanueva, L., Bale, N. J., Offre, P., Reichart, G.-J., & Schouten, S. (2024a). Controls on the composition of hydroxylated isoprenoidal glycerol dialkyl glycerol tetraethers (isoGDGTs) in cultivated ammonia-oxidizing Thaumarchaeota. *Biogeosciences*, 21(21), 4875–4888. <https://doi.org/10.5194/bg-21-4875-2024>
- Varma, D., Yedema, Y. W., Peterse, F., Reichart, G.-J., Sinninghe Damsté, J. S., & Schouten, S. (2025). Impact of terrestrial organic matter input on distributions of hydroxylated isoprenoidal GDGTs in marine sediments: Implications for OH-isoGDGT-based temperature proxies. *Organic Geochemistry*, 206, 105010. <https://doi.org/10.1016/j.orggeochem.2025.105010>
- Villanueva, L., Schouten, S., & Sinninghe Damsté, J. S. (2015). Depth-related distribution of a key gene of the tetraether lipid biosynthetic pathway in marine Thaumarchaeota. *Environmental Microbiology*, 17(10), 3527–3539. <https://doi.org/10.1111/1462-2920.12508>
- Villanueva, L., Schouten, S., & Sinninghe Damsté, J. S. (2017). Phylogenomic analysis of lipid biosynthetic genes of Archaea shed light on the 'lipid divide'. *Environmental Microbiology*, 19(1), 54–69. <https://doi.org/10.1111/1462-2920.13361>
- Villanueva, L., Sinninghe Damsté, J. S., & Schouten, S. (2014). A re-evaluation of the archaeal membrane lipid biosynthetic pathway. *Nature Reviews Microbiology*, 12(6), 438–448. <https://doi.org/10.1038/nrmicro3260>
- Viola, J., Woerner, L., Hinrichs, K.-U., & Laepple, T. (2025). Microscale Alkenone Heterogeneity and Replicability of Ultra-High-Resolution Temperature Records from Marine Sediments. *EGU sphere*. <https://doi.org/10.5194/egusphere-2025-5089>
- Vorath, M.-E., Müller, J., Cárdenas, P., Opel, T., Mieruch, S., Esper, O., et al. (2023). Deglacial and Holocene sea-ice and climate dynamics in the Bransfield Strait, northern Antarctic Peninsula. *Climate of the Past*, 19(5), 1061–1079. <https://doi.org/10.5194/cp-19-1061-2023>
- Wakeham, S. G., Amann, R., Freeman, K. H., Hopmans, E. C., Jørgensen, B. B., Putnam, I. F., et al. (2007). Microbial ecology of the stratified water column of the Black Sea as revealed by a comprehensive biomarker study. *Organic Geochemistry*, 38(12), 2070–2097. <https://doi.org/10.1016/j.orggeochem.2007.08.003>
- Wakeham, S. G., Hopmans, E. C., Schouten, S., & Sinninghe Damsté, J. S. (2004). Archaeal lipids and anaerobic oxidation of methane in euxinic water columns: A comparative study of the Black Sea and Cariaco Basin. *Chemical Geology*, 205(3–4), 427–442. <https://doi.org/10.1016/j.chemgeo.2003.12.024>
- Wakeham, S. G., Lewis, C. M., Hopmans, E. C., Schouten, S., & Sinninghe Damsté, J. S. (2003). Archaea mediate anaerobic oxidation of methane in deep euxinic waters of the Black Sea. *Geochimica et Cosmochimica Acta*, 67(7), 1359–1374. [https://doi.org/10.1016/s0016-7037\(02\)01220-6](https://doi.org/10.1016/s0016-7037(02)01220-6)
- Wakeham, S. G., Turich, C., Schubotz, F., Podlaska, A., Li, X. N., Varela, R., et al. (2012). Biomarkers, chemistry and microbiology show chemoautotrophy in a multilayer chemocline in the Cariaco Basin. *Deep Sea Research Part I: Oceanographic Research Papers*, 63, 133–156. <https://doi.org/10.1016/j.dsr.2012.01.005>
- Wang, H., Liu, W., Lu, H., Zhang, Y., Liang, Y., He, Y., et al. (2023). Oxygenated deep waters fed early Atlantic overturning circulation upon Antarctic glaciation. *Nature Geoscience*, 16(11), 1014–1019. <https://doi.org/10.1038/s41561-023-01292-2>
- Wang, J.-X., Wei, Y., Wang, P., Hong, Y., & Zhang, C. L. (2015). Unusually low TEX₈₆ values in the transitional zone between Pearl River estuary and coastal South China Sea: Impact of changing archaeal community composition. *Chemical Geology*, 402, 18–29. <https://doi.org/10.1016/j.chemgeo.2015.03.002>
- Wegener, G., Laso-Pérez, R., Orphan, V. J., & Boetius, A. (2022). Anaerobic Degradation of Alkanes by Marine Archaea. *Annual Review of Microbiology*, 76(1), 553–577. <https://doi.org/10.1146/annurev-micro-111021-045911>
- Wei, B., Jia, G., Hefter, J., Kang, M., Park, E., Wang, S., & Mollenhauer, G. (2020). Comparison of the U^{K'}₃₇, LDI, TEX₈₆^H, and RI-OH temperature proxies in sediments from the northern shelf of the South China Sea. *Biogeosciences*, 17(17), 4489–4508. <https://doi.org/10.5194/bg-17-4489-2020>
- Weijers, J. W. H., Lim, K. L. H., Aquilina, A., Sinninghe Damsté, J. S., & Pancost, R. D. (2011). Biogeochemical controls on glycerol dialkyl glycerol tetraether lipid distributions in sediments characterized by diffusive methane flux. *Geochemistry, Geophysics, Geosystems*, 12(10). <https://doi.org/10.1029/2011GC003724>
- Weijers, J. W. H., Schouten, S., Spaargaren, O. C., & Sinninghe Damsté, J. S. (2006). Occurrence and distribution of tetraether membrane lipids in soils: Implications for the use of the TEX₈₆ proxy and the BIT index. *Organic Geochemistry*, 37(12), 1680–1693. <https://doi.org/10.1016/j.orggeochem.2006.07.018>

- Weijers, J. W. H., Schouten, S., van den Donker, J. C., Hopmans, E. C., & Sinninghe Damsté, J. S. (2007). Environmental controls on bacterial tetraether membrane lipid distribution in soils. *Geochimica et Cosmochimica Acta*, 71(3), 703–713. <https://doi.org/10.1016/j.gca.2006.10.003>
- Wijker, R. S., Sessions, A. L., Fuhrer, T., & Phan, M. (2019). $^2\text{H}/^1\text{H}$ variation in microbial lipids is controlled by NADPH metabolism. *Proceedings of the National Academy of Sciences*, 116(25), 12173–12182. <https://doi.org/10.1073/pnas.1818372116>
- Wittenborn, A. K., Bauersachs, T., Hassenrück, C., Käding, K., Wäge-Reccioni, J., Jürgens, K., et al. (2023). *Nitrosopumilus* as main source of isoprenoid glycerol dialkyl glycerol tetraether lipids in the central Baltic Sea. *Frontiers in Microbiology*, 14, 1216130. <https://doi.org/10.3389/fmicb.2023.1216130>
- Wittenborn, A. K., Radtke, H., Dutheil, C., Arz, H. W., & Kaiser, J. (2022). A downcore calibration of the $\text{TEX}_{86}^{\text{L}}$ temperature proxy for the Baltic Sea. *Continental Shelf Research*, 251, 104875. <https://doi.org/10.1016/j.csr.2022.104875>
- Woelders, L., Vellekoop, J., Weltje, G. J., de Nooijer, L., Reichart, G.-J., Peterse, F., et al. (2018). Robust multi-proxy data integration, using late Cretaceous paleotemperature records as a case study. *Earth and Planetary Science Letters*, 500, 215–224. <https://doi.org/10.1016/j.epsl.2018.08.010>
- Woese, C. R., & Fox, G. E. (1977). Phylogenetic structure of the prokaryotic domain: The primary kingdoms. *Proceedings of the National Academy of Sciences*, 74(11), 5088–5090. <https://doi.org/10.1073/pnas.74.11.5088>
- Woese, C. R., Magrum, L. J., & Fox, G. E. (1978). Archaeobacteria. *Journal of Molecular Evolution*, 11(3), 245–252. <https://doi.org/10.1007/BF01734485>
- Wörmer, L., Lipp, J. S., & Hinrichs, K.-U. (2015). Comprehensive analysis of microbial lipids in environmental samples through HPLC-MS protocols. In T. J. McGenity, K. N. Timmis, & B. Nogales (Eds.), *Hydrocarbon and Lipid Microbiology Protocols* (pp. 289–317). Springer. https://doi.org/10.1007/8623_2015_183
- Wörmer, L., Lipp, J. S., Schröder, J. M., & Hinrichs, K.-U. (2013). Application of two new LC-ESI-MS methods for improved detection of intact polar lipids (IPLs) in environmental samples. *Organic Geochemistry*, 59, 10–21. <https://doi.org/10.1016/j.orggeochem.2013.03.004>
- Wubben, E., Spiering, B. R., Veenstra, T., Bos, R., Wang, Z., van Dijk, J., et al. (2024). Tropical warming and intensification of the West African monsoon during the Miocene climatic optimum. *Paleoceanography and Paleoclimatology*, 39(5), e2023PA004767. <https://doi.org/10.1029/2023PA004767>
- Wuchter, C., Abbas, B., Coolen, M. J. L., Herfort, L., van Bleijswijk, J., Timmers, P., et al. (2006a). Archaeal nitrification in the ocean. *Proceedings of the National Academy of Sciences*, 103(33), 12317–12322. <https://doi.org/10.1073/pnas.0600756103>
- Wuchter, C., Schouten, S., Boschker, H. T. S., & Sinninghe Damsté, J. S. (2003). Bicarbonate uptake by marine Crenarchaeota. *FEMS Microbiology Letters*, 219(2), 203–207. [https://doi.org/10.1016/s0378-1097\(03\)00060-0](https://doi.org/10.1016/s0378-1097(03)00060-0)
- Wuchter, C., Schouten, S., Coolen, M. J. L., & Sinninghe Damsté, J. S. (2004). Temperature-dependent variation in the distribution of tetraether membrane lipids of marine Crenarchaeota: Implications for TEX_{86} paleothermometry. *Paleoceanography*, 19(4), PA4028. <https://doi.org/10.1029/2004pa001041>
- Wuchter, C., Schouten, S., Wakeham, S. G., & Sinninghe Damsté, J. S. (2005). Temporal and spatial variation in tetraether membrane lipids of marine Crenarchaeota in particulate organic matter: Implications for TEX_{86} paleothermometry. *Paleoceanography*, 20(3), PA3013. <https://doi.org/10.1029/2004PA001110>
- Wuchter, C., Schouten, S., Wakeham, S. G., & Sinninghe Damsté, J. S. (2006b). Archaeal tetraether membrane lipid fluxes in the northeastern Pacific and the Arabian Sea: Implications for TEX_{86} paleothermometry. *Paleoceanography*, 21(4), PA4208. <https://doi.org/10.1029/2006pa001279>
- Xiao, R., Xing, L., Chen, J., Wang, Y., Zhong, G., Zhou, Y., et al. (2023a). Spatial discrepancy of hydrodynamics-driven impacts on organic biomarkers deposition and U^{K}_{37} and TEX_{86} temperature proxies applications. *Global Biogeochemical Cycles*, 37(4), e2022GB007648. <https://doi.org/10.1029/2022GB007648>
- Xiao, W., Peng, X., Xu, Y., Chen, Y., Yao, W., Ta, K., et al. (2026). Global distribution of marine bacterial BrGDGTs in sediments: Patterns and implications. *Geochimica et Cosmochimica Acta*, 413, 18–32. <https://doi.org/10.1016/j.gca.2025.12.004>
- Xiao, W., Xu, Y., Zhang, C., Lin, J., Wu, W., Lü, X., et al. (2023b). Disentangling effects of sea surface temperature and water depth on hydroxylated isoprenoid GDGTs: Insights from the Hadal zone and global sediments. *Geophysical Research Letters*, 50(15), e2023GL103109. <https://doi.org/10.1029/2023GL103109>
- Xie, S., Lipp, J. S., Wegener, G., Ferdelman, T. G., & Hinrichs, K.-U. (2013). Turnover of microbial lipids in the deep biosphere and growth of benthic archaeal populations. *Proceedings of the National Academy of Sciences*, 110(15), 6010–6014. <https://doi.org/10.1073/pnas.1218569110>
- Xie, S., Liu, X.-L., Schubotz, F., Wakeham, S. G., & Hinrichs, K.-U. (2014). Distribution of glycerol ether lipids in the oxygen minimum zone of the Eastern Tropical North Pacific Ocean. *Organic Geochemistry*, 71, 60–71. <https://doi.org/10.1016/j.orggeochem.2014.04.006>
- Yamamoto, M., Shimamoto, A., Fukuhara, T., Tanaka, Y., & Ishizaka, J. (2012). Glycerol dialkyl glycerol tetraethers and TEX_{86} index in sinking particles in the western North Pacific. *Organic Geochemistry*, 53, 52–62. <https://doi.org/10.1016/j.orggeochem.2012.04.010>
- Yang, Y., Gao, C., Dang, X., Ruan, X., Lü, X., Xie, S., et al. (2018). Assessing hydroxylated isoprenoid GDGTs as a paleothermometer for the tropical South China Sea. *Organic Geochemistry*, 115, 156–165. <https://doi.org/10.1016/j.orggeochem.2017.10.014>
- Yang, Y., Zhang, C., Lenton, T. M., Yan, X., Zhu, M., Zhou, M., et al. (2021). The evolution pathway of ammonia-oxidizing archaea shaped by major geological events. *Molecular Biology and Evolution*.
- Yao, W., Zhang, W., He, W., Xiao, W., Chen, Y., Zhu, Y., et al. (2023). Lipidomic chemotaxonomy aligned with phylogeny of Halobacteria. *Frontiers in Microbiology*, 14, 1297600. <https://doi.org/10.3389/fmicb.2023.1297600>
- Yoshinaga, M. Y., Kellermann, M. Y., Rossel, P. E., Schubotz, F., Lipp, J. S., & Hinrichs, K.-U. (2011). Systematic fragmentation patterns of archaeal intact polar lipids by high-performance liquid chromatography/electrospray ionization ion-trap mass spectrometry: Fragmentation patterns of archaeal intact polar lipids. *Rapid Communications in Mass Spectrometry*, 25(23), 3563–3574. <https://doi.org/10.1002/rcm.5251>
- Yoshinaga, M. Y., Lazar, C. S., Elvert, M., Lin, Y.-S., Zhu, C., Heuer, V. B., et al. (2015). Possible roles of uncultured archaea in carbon cycling in methane-seep sediments. *Geochimica et Cosmochimica Acta*, 164, 35–52. <https://doi.org/10.1016/j.gca.2015.05.003>
- Yu, T., Wu, W., Liang, W., Lever, M. A., Hinrichs, K.-U., & Wang, F. (2018). Growth of sedimentary *Bathymarchaeota* on lignin as an energy source. *Proceedings of the National Academy of Sciences*, 115(23), 6022–6027. <https://doi.org/10.1073/pnas.1718854115>
- Zachos, J. C., Schouten, S., Bohaty, S., Quattlebaum, T., Sluijs, A., Brinkhuis, H., et al. (2006). Extreme warming of mid-latitude coastal ocean during the Paleocene-Eocene Thermal Maximum: Inferences from TEX_{86} and isotope data. *Geology*, 34(9), 737–740. <https://doi.org/10.1130/G22522.1>
- Zehnle, H. (2023). *Exploring the upper temperature limit and biosignatures of archaea and bacteria involved in anaerobic hydrocarbon degradation* (PhD Thesis). Universität Bremen. Retrieved from <https://media.suub.uni-bremen.de/handle/elib/7473>

- Zell, C., Kim, J.-H., Hollander, D., Lorenzoni, L., Baker, P., Silva, C. G., et al. (2014). Sources and distributions of branched and isoprenoid tetraether lipids on the Amazon shelf and fan: Implications for the use of GDGT-based proxies in marine sediments. *Geochimica et Cosmochimica Acta*, 139, 293–312. <https://doi.org/10.1016/j.gca.2014.04.038>
- Zell, C., Kim, J.-H., Moreira-Turcq, P., Abril, G., Hopmans, E. C., Bonnet, M.-P., et al. (2013). Disentangling the origins of branched tetraether lipids and crenarchaeol in the lower Amazon River: Implications for GDGT-based proxies. *Limnology and Oceanography*, 58(1), 343–353. <https://doi.org/10.4319/lo.2013.58.1.0343>
- Zeng, Z., Chen, H., Yang, H., Chen, Y., Yang, W., Feng, X., et al. (2022). Identification of a protein responsible for the synthesis of archaeal membrane-spanning GDGT lipids. *Nature Communications*, 13(1), 1545. <https://doi.org/10.1038/s41467-022-29264-x>
- Zeng, Z., Liu, X.-L., Farley, K. R., Wei, J. H., Metcalf, W. W., Summons, R. E., & Welander, P. V. (2019). GDGT cyclization proteins identify the dominant archaeal sources of tetraether lipids in the ocean. *Proceedings of the National Academy of Sciences*, 116(45), 22505–22511. <https://doi.org/10.1073/pnas.1909306116>
- Zeng, Z., Liu, X.-L., Wei, J. H., Summons, R. E., & Welander, P. V. (2018). Caldito-linked membrane lipids are required for acid tolerance in *Sulfolobus acidocaldarius*. *Proceedings of the National Academy of Sciences*, 115(51), 12932–12937. <https://doi.org/10.1073/pnas.1814048115>
- Zhang, D., & Poulter, C. D. (1993). Biosynthesis of archaeobacterial ether lipids. Formation of ether linkages by prenyltransferases. *Journal of the American Chemical Society*, 115(4), 1270–1277. <https://doi.org/10.1021/ja00057a008>
- Zhang, T., He, W., Liang, Q., Zheng, F., Xiao, X., Zeng, Z., et al. (2023). Lipidomic diversity and proxy implications of archaea from cold seep sediments of the South China Sea. *Frontiers in Microbiology*, 14, 1241958. <https://doi.org/10.3389/fmicb.2023.1241958>
- Zhang, Y. G., Pagani, M., & Liu, Z. (2014). A 12-million-year temperature history of the tropical Pacific Ocean. *Science*, 344(6179), 84–87. <https://doi.org/10.1126/science.1246172>
- Zhang, Y. G., Pagani, M., & Wang, Z. (2016). Ring index: A new strategy to evaluate the integrity of TEX₈₆ paleothermometry. *Paleoceanography*, 31(2), 220–232. <https://doi.org/10.1002/2015PA002848>
- Zhang, Y. G., Zhang, C. L., Liu, X.-L., Li, L., Hinrichs, K.-U., & Noakes, J. E. (2011). Methane index: A tetraether archaeal lipid biomarker indicator for detecting the instability of marine gas hydrates. *Earth and Planetary Science Letters*, 307(3–4), 525–534. <https://doi.org/10.1016/j.epsl.2011.05.031>
- Zheng, F., Yao, W., He, W., Zhang, W., Chen, Y., Chen, H., et al. (2025). A comprehensive database for high-throughput identification of archaeal lipids using high-resolution mass spectrometry. *Nature Communications*, 17(1), 588. <https://doi.org/10.1038/s41467-025-67286-3>
- Zhou, A., Weber, Y., Chiu, B. K., Elling, F. J., Cobban, A. B., Pearson, A., & Leavitt, W. D. (2020). Energy flux controls tetraether lipid cyclization in *Sulfolobus acidocaldarius*. *Environmental Microbiology*, 22(1), 343–353. <https://doi.org/10.1111/1462-2920.14851>
- Zhou, J., & Dong, L. (2024). Molecular dynamics simulations reveal methylation in Me-GDGTs as a microbial low-temperature adaptation. *Chemical Geology*, 644, 121844. <https://doi.org/10.1016/j.chemgeo.2023.121844>
- Zhou, Z., St. John, E., Anantharaman, K., & Reysenbach, A.-L. (2022). Global patterns of diversity and metabolism of microbial communities in deep-sea hydrothermal vent deposits. *Microbiome*, 10(1), 241. <https://doi.org/10.1186/s40168-022-01424-7>
- Zhu, C., Lipp, J. S., Wörmer, L., Becker, K. W., Schröder, J., & Hinrichs, K.-U. (2013). Comprehensive glycerol ether lipid fingerprints through a novel reversed phase liquid chromatography–mass spectrometry protocol. *Organic Geochemistry*, 65, 53–62. <https://doi.org/10.1016/j.orggeochem.2013.09.012>
- Zhu, C., Meador, T. B., Dummman, W., & Hinrichs, K.-U. (2014b). Identification of unusual butanetriol dialkyl glycerol tetraether and pentanetriol dialkyl glycerol tetraether lipids in marine sediments. *Rapid Communications in Mass Spectrometry*, 28(4), 332–338. <https://doi.org/10.1002/rcm.6792>
- Zhu, C., Wakeham, S. G., Elling, F. J., Basse, A., Mollenhauer, G., Versteegh, G. J. M., et al. (2016). Stratification of archaeal membrane lipids in the ocean and implications for adaptation and chemotaxonomy of planktonic archaea. *Environmental Microbiology*, 18(12), 4324–4336. <https://doi.org/10.1111/1462-2920.13289>
- Zhu, C., Weijers, J. W. H., Wagner, T., Pan, J.-M., Chen, J.-F., & Pancost, R. D. (2011). Sources and distributions of tetraether lipids in surface sediments across a large river-dominated continental margin. *Organic Geochemistry*, 42(4), 376–386. <https://doi.org/10.1016/j.orggeochem.2011.02.002>
- Zhu, C., Yoshinaga, M. Y., Peters, C. A., Liu, X.-L., Elvert, M., & Hinrichs, K.-U. (2014a). Identification and significance of unsaturated archaeal tetraether lipids in marine sediments. *Rapid Communications in Mass Spectrometry*, 28(10), 1144–1152. <https://doi.org/10.1002/rcm.6887>
- Zhu, Q.-Z., Elvert, M., Meador, T. B., Becker, K. W., Heuer, V. B., & Hinrichs, K. (2021). Stable carbon isotopic compositions of archaeal lipids constrain terrestrial, planktonic, and benthic sources in marine sediments. *Geochimica et Cosmochimica Acta*, 307, 319–337. <https://doi.org/10.1016/j.gca.2021.04.037>
- Zhu, Q.-Z., Elvert, M., Meador, T. B., Schröder, J. M., Doeana, K. D., Becker, K. W., et al. (2024). Comprehensive molecular-isotopic characterization of archaeal lipids in the Black Sea water column and underlying sediments. *Geobiology*, 22(2), e12589. <https://doi.org/10.1111/gbi.12589>
- Zhuang, G.-C., Elling, F. J., Nigro, L. M., Samarkin, V., Joye, S. B., Teske, A., & Hinrichs, K.-U. (2016). Multiple evidence for methylotrophic methanogenesis as the dominant methanogenic pathway in hypersaline sediments from the Orca Basin, Gulf of Mexico. *Geochimica et Cosmochimica Acta*, 187, 1–20. <https://doi.org/10.1016/j.gca.2016.05.005>
- Zuffa, S., Schmid, R., Bauermeister, A., P. Gomes, P. W., Caraballo-Rodriguez, A. M., El Abiead, Y., et al. (2024). microbeMASST: A taxonomically informed mass spectrometry search tool for microbial metabolomics data. *Nature Microbiology*, 9(2), 336–345. <https://doi.org/10.1038/s41564-023-01575-9>