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Development of a regional glycerol dialkyl glycerol tetraether (GDGT)–temperature calibration for Antarctic and sub-Antarctic lakes

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ABSTRACT

A regional network of quantitative reconstructions of past climate variability is required to test climate models. In recent studies, temperature calibration models based on the relative abundances of sedimentary glycerol dialkyl glycerol tetraethers (GDGTs) have enabled past temperature reconstructions in both marine and terrestrial environments. Nevertheless, to date these methods have not been widely applied in high latitude environments due to poor performance of the GDGT–temperature calibrations at lower temperatures. To address this we studied 32 lakes from Antarctica, the sub-Antarctic Islands and Southern Chile to: 1) quantify their GDGT composition and investigate the environmental controls on GDGT composition; and 2) develop a GDGT–temperature calibration model for inferring past temperatures from Antarctic and sub-Antarctic lakes. GDGTs were found in all 32 lakes studied and in 31 lakes branched GDGTs (brGDGTs) were the dominant compounds. Statistical analyses of brGDGT composition in relation to temperature, pH, conductivity and water depth showed that the composition of brGDGTs is strongly correlated with mean summer air temperature (MSAT). This enabled the development of the first regional brGDGT–temperature calibration for use in Antarctic and sub-Antarctic lakes using four brGDGT compounds (GDGT-Ib, GDGT-II, GDGT-III and GDGT-IIIb). A key discovery was that GDGT-IIIb is of particular importance in cold lacustrine environments. The addition of this compound significantly improved the model's performance from $r^2 = 0.67$, RMSEP-LOO (leave-one-out) = 2.23 °C, RMSEP-H (h-block) = 2.37 °C when applying the re-calibrated global GDGT–temperature calibration to our Antarctic dataset to $r^2 = 0.83$, RMSEP-LOO = 1.68 °C, RMSEP-H = 1.65 °C for our new Antarctic calibration. This shows that Antarctic and sub-Antarctic, and possibly other high latitude, palaeotemperature reconstructions should be based on a regional GDGT–temperature calibration where specific compounds can be identified and included to improve model performance. Finally, downcore temperature reconstructions using the new Antarctic brGDGT–temperature calibration were tested in sub-Antarctic Fan Lake from South Georgia providing a proof of concept for the new calibration model in the Southern Hemisphere.

1. Introduction

Previous studies of past climates in high-latitude regions have used a range of biological proxies including changes in accumulation rates and species composition of pollen, diatoms, pigments and chironomids to give indirect qualitative or quantitative inferences about past environmental changes (e.g., Anderson et al., 2001; Verleyen et al., 2003; Hodgson et al., 2005; Rolland et al., 2009; Watcham et al., 2011; Strother et al., 2015). Many of these proxies respond to a range of environmental controls, including pH, salinity or atmospheric circulation, all of which can influence their ability to accurately quantify past changes in temperature (Shanahan et al., 2013). Moreover, in the harsh Antarctic environment, palaeoclimate techniques are restricted due to the biological proxies being limited or absent, so there is a real need for a robust method to quantify temperature. This is particularly important in Antarctic lakes where quantitative temperature reconstructions using biogeochemical proxies in lake sediment cores will enable a

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substantial improvement in our understanding of past atmospheric temperature at low altitudes without the complicating factors of changing ocean currents (which limit the application of marine-based palaeothermometry through redistributing heat e.g., Kim et al., 2012) and high altitude temperature effects (which apply to most ice core reconstructions e.g., Mulvaney et al., 2012).

One such approach is the application of glycerol dialkyl glycerol tetraethers (GDGTs). Several studies have used changes in the relative abundance of GDGTs in ocean sediments (e.g., Schouten et al., 2002; Kim et al., 2010; Tierney and Tingley, 2014), soils (e.g., Weijers et al., 2007a; Peterse et al., 2012) and lake sediments (e.g., Powers et al., 2005; Tierney et al., 2010; Pearson et al., 2011; Loomis et al., 2012) for quantitatively reconstructing past temperature. GDGTs are cell membrane lipids found in archaea and bacteria and their structure strongly depends on growth temperature (Schouten et al., 2002; Weijers et al., 2006). More specifically, the number of cyclopentane rings in the GDGT structure is a key factor in the adaptation to temperature change (Gliozzi et al., 1983; Uda et al., 2001; Schouten et al., 2002). To date GDGTs have only been studied in seven Antarctic and sub-Antarctic lakes as part of the Pearson et al. (2011) global calibration model. In these few sites the GDGT–temperature relationship does not appear to be as strong as the global relationship, suggesting a need to expand upon and further investigate the environmental controls on GDGT composition in Antarctic lakes.

1.1. GDGTs in lacustrine environments

Powers et al. (2004, 2005) first investigated the use of GDGTs in lacustrine environments, developing a lacustrine variation of the marine TEX_{86} index, and demonstrated its potential as a temperature proxy in large lakes. However, its dependence on isoprenoid GDGTs (isoGDGTs), which are frequently in low abundance in lakes, means TEX_{86} is often not applicable. The Branched Isoprenoid Tetraether (BIT) index is the ratio of branched GDGTs (brGDGTs) to isoGDGTs which can be used to identify lakes with a high proportion of brGDGTs and thus where the TEX_{86} index will be unreliable (e.g., BIT $>$ 0.5; Hopmans et al., 2004; Weijers et al., 2006; Blaga et al., 2009). This interpretation must be approached with caution as Weijers et al. (2007a), Tierney et al. (2010) and Pearson et al. (2011) all found that the BIT value was predominantly related to low concentrations of Crenarchaeol, an isoGDGT, rather than a high abundance of brGDGTs.

Alternatively, the soil MBT/CBT index, developed by Weijers et al. (2007a) uses brGDGTs which often dominate the GDGT composition in lacustrine environments. Although several studies have applied this MBT/CBT soil index in lakes (e.g., Sinninghe Damsté et al., 2009; Tierney et al., 2010; Sun et al., 2011; Loomis et al., 2012; Naeher et al., 2014), it can underestimate measured temperatures by up to 15 °C.

The limitations of TEX_{86} and MBT/CBT indices has led to the development of GDGT–temperature calibrations specific to lacustrine environments, including a global brGDGT–temperature regression model by Pearson et al. (2011) and regional models for East Africa by Tierney et al. (2010) and Loomis et al. (2012). Pearson et al. (2011) used the fractional abundances of brGDGTs to develop a global calibration using 85 lakes from the Scandinavian Arctic to Antarctica and applied best subsets regression to select a subset of brGDGT compounds with optimal predictive properties for mean summer air temperature (MSAT) (Eq. (1)).

$$\text{MSAT} = 20.9 + (98.1 \times \text{GDGT-Ib}) - (12.0 \times \text{GDGT-II}) - (20.5 \times \text{GDGT-III}) \quad (1)$$

This global calibration has a high accuracy and precision ($r^2 = 0.88$, RMSE $= 2.0$ °C, RMSEP $= 2.1$ °C) and is not significantly influenced by pH, conductivity or water depth. Naeher et al. (2014) applied the model to Lake Rotsee, Switzerland and found good correlation between reconstructed and measured temperatures.

Loomis et al. (2012) developed a regional East African brGDGT–temperature calibration for mean annual air temperature (MAAT) (Eq. (2)) adding 70 lakes to the 41 studied by Tierney et al. (2010), and adding one additional brGDGT compound (GDGT-IIc) to those used by Pearson et al. (2011).

$$\text{MAAT} = 22.77 - (35.58 \times \text{GDGT-III}) - (12.88 \times \text{GDGT-II}) - (418.53 \times \text{GDGT-IIc}) + (86.43 \times \text{GDGT-Ib}) \quad (2)$$

Although GDGT-IIc does not have a significant relationship with temperature in the global dataset of Pearson et al. (2011), it does improve model performance in the East African regional model. Loomis et al. (2012) concluded that regional calibrations had better predictive ability compared with global calibrations. Regional calibrations can only be achieved where temperature gradients are sufficiently large. In the East Africa dataset this is achieved by sampling lakes along an altitudinal gradient.

Sinninghe Damsté et al. (2012) applied both the Tierney et al. (2010) and the Pearson et al. (2011) brGDGT–temperature calibrations in Lake Challa, equatorial Africa, finding that the temperature difference between the Last Glacial Maximum and the Holocene for both calibrations was consistent with previous temperature reconstructions by Powers et al. (2005), Weijers et al. (2007b) and Tierney et al. (2008). More recently, Woltering et al. (2014) applied ten different GDGT–temperature calibrations, including both soil and lake calibrations, to a core from Lake McKenzie, Australia. They showed that although all calibrations indicated significantly lower temperatures during the last glacial period, the choice of calibration affected both the trend and absolute values of the reconstructed temperatures, highlighting the need for careful choice of calibration model (Woltering et al., 2014, Fig. 4).

Equation (1) provides the best fit calibration with minimum prediction error across a wide range of temperatures for Pearson et al.'s (2011) global dataset, but the model included only six sites with MSAT below 5 °C and none below 1.5 °C. As a consequence, it performs relatively poorly at low temperatures and overestimated MSAT in this part of the gradient (Pearson et al., 2011, Fig. 7b).

To address this limitation we studied 32 lakes from Antarctica, the sub-Antarctic Islands and Southern Chile, adding 26 new lakes to the high latitude Southern Hemisphere lakes studied by Pearson et al. (2011). Combining the two datasets we had a total of 37 samples including five replicate samples from sites included in Pearson et al. (2011) and re-sampled as part of this study. The aims of this paper are to: 1) quantify the GDGT composition of lake surface sediments and investigate the environmental controls on GDGT composition in Antarctic and sub-Antarctic lakes; 2) develop a brGDGT–temperature calibration for inferring past temperatures from Antarctic and sub-Antarctic lakes; and 3) test the calibration on a lake-sediment core from the sub-Antarctic.

2. Materials and methods

2.1. Study locations

Surface sediments (top 0–2 cm) from 32 lakes from Antarctica, the sub-Antarctic Islands and Southern Chile (Fig. 1) were collected using a UWITEC surface gravity corer during several field campaigns in the Southern Hemisphere spring–summer season. Sites spanned a range of MAAT from −11.8 to 6.1 °C and MSAT (December to February) from −2.2 to 10.3 °C. The sites also covered a range of pH (4.5 to 9.8), conductivity (0.01 to 7.38 mS cm^{-1}) and water depths (0.5 to 55 m). A summary of the temperature and limnological data for lakes in each region is listed in Table 1 and outlined for each individual lake in Supplementary Table S1.