A rapid lake-shallowing event terminated preservation of the Miocene Clarkia Fossil Konservat-Lagerstätte (Idaho, USA)

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Extended Methods

Sample Collection: Sediment samples were collected at ca. 10–15 cm intervals along the Clarkia lacustrine sequence from a newly exposed trench at the outcrop of the P-33 type locality at the St. Maries River Valley in northern Idaho, USA (Smiley et al., 1975; Smiley and Rember 1981, 1985; Yang, 1993; Yang et al., 1995; Yang and Huang, 2003) in August 2014 (Fig. 1; Table DR1). Fine powder was obtained by scraping the portion of sedimentary rock where no macrofossil was visible. The lower (L) series (L1–L11) samples were collected between the lower volcanic ash bed (i.e., Unit 2c of Smiley and Rember, 1985) and the middle volcanic ash layer (Unit 4 of
Smiley and Rember, 1985). The two uppermost L series samples, L10 and L11, were from the transitional layer (Unit 3 of Smiley and Rember, 1985). The upper (U) series samples (U1–U9) were collected above the middle ash layer, with U1–U6 from Unit 5a and U7–U9 from Unit 5c of Smiley and Rember (1985). Unit 5b is a volcanic ash layer with a thickness of ca. 10 cm (Fig. 1; Table DR1). The excellent preservation of fossil leaves and insects from the lower unoxidized stratigraphic horizons is represented by the original coloration of leaves (Smiley et al., 1975), structural colors of insects (McNamara et al., 2012), leaf ultra-structures (Niklas et al., 1985), and a suite of ancient biomolecules such as flavonoids (Giannasi and Niklas, 1981; Rieseberg and Soltis, 1987), lignin (Logan et al., 1993), polysaccharides (Yang et al., 2005), terpenoids (Otto et al., 2003), lipids (Logan and Eglinton, 1994; Huang et al., 1995), and possible DNA and amino acids (Golenberg et al., 1990; Soltis et al., 1992).

**Total organic carbon (TOC) content analysis:** TOC content of 3 typical samples (L1, L10, and U1) from the 3 units (Units 2d, 3, and 5) was determined according to Wei et al. (2012): after removing visible plant residue, ca. 3 g freeze dried sample was ground in an agate mortar, sieved through a 100 mesh screen and homogenized. It was then soaked in 2 M HCl for 24 h to exclude inorganic carbon and washed with distilled water until pH > 6. The samples were then dried at 40 °C and re-homogenized. Finally, an aliquot (ca. 30–70 mg) was analyzed using an Elemental Analyzer instrument (Vario EL III, Hanau, Germany).

**Lipid extraction and purification:** Each sediment sample was homogenized using a mortar and pestle after freeze-drying, and then 1–2 g of the fine powder was
extracted ultrasonically using MeOH:Dichloromethane (DCM) (1:1, v/v) for 5 times. Subsequently, the total lipid extract was dried under N₂, and fractionated over an activated silica gel column into an apolar and a polar fraction using hexane and MeOH:DCM (1:1 v/v), respectively. The apolar fraction with saturated hydrocarbons was further purified by a urea-adduct process to remove branched/cyclic alkanes from \textit{n}-alkanes. The polar fraction was filtered through a 0.22 \textmu m PTFE filter after adding a known amount of C_{46} glycerol dialkyl glycerol tetraether (GDGT) internal standard (Huguet et al., 2006).

\textbf{Isotopic analysis of \textit{n}-alkanes:} The hydrogen isotope compositions (δD values) of long-chain \textit{n}-alkanes for 11 samples were measured on a coupled gas chromatography–isotope ratio mass spectrometry (GC–IRMS) system at the stable isotope laboratory of the Institute of Earth Environment, Chinese Academy of Sciences (IEECAS) in Xi'an, China, following Cao et al. (2012). Separation of individual long-chain \textit{n}-alkanes was achieved using a Trace GC UltraTM gas chromatograph (Thermo Scientific) equipped with an HP-1 MS column (60 m × 0.32 mm i.d. × 0.25 \textmu m). Injection was performed in splitless mode at 270 °C. The temperature program of the GC oven was as follows: isothermal at 40 °C for 1 min, increased at 10 °C/min to 150 °C, further increased at 6 °C/min to 310 °C, and finally held for 20 min isothermally. The carrier gas was helium with a flow rate of 1 ml/min. After GC separation, individual long-chain \textit{n}-alkanes were pyrolyzed into H₂ gas quantitatively at 1430 °C in an alumina tube (0.5 mm i.d., 320 mm length), and subsequently the generated H₂ gas was transported into the ion source of the IRMS for
δD measurements. The H$_3^+$ factor was calculated daily using H$_2$ reference gas, and the variability was < 0.1 ppm/nA/day. The δD value of a standard mixture of n-alkane homologues (n-C$_{21}$, n-C$_{25}$, n-C$_{27}$, n-C$_{29}$, n-C$_{31}$, and n-C$_{33}$) was measured every four samples and the standard deviation for individual n-alkanes was less than 3‰. Selected samples were analyzed in duplicate and the standard deviation for n-C$_{27}$, n-C$_{29}$, and n-C$_{31}$ was less than 4‰ (Table DR1). All reported δD values (‰) are relative to VSMOW (0‰).

**GDGT measurements:** GDGTs of the 20 samples were measured on a high performance liquid chromatography/atmospheric pressure chemical ionization-mass spectrometry (HPLC/APCI-MS) system (Shimadzu LC-MS 8030) at IEECAS according to a method modified from Schouten et al. (2007). The polar fraction of each sample was dissolved in 1500 μl of n-hexane, and generally 5 μl was injected. Separation of GDGTs was obtained on an Inertsil CN-3 column (250 mm × 4.6 mm, 3 μm; GL Sciences Inc.) at 40 °C using n-hexane:isopropanol (9:1) and n-hexane as elutes for pump A and pump B, respectively. The eluting gradient for B was as follows: 96% (0–10 min), decreased linearly to 87% (10–40 min), decreased linearly to 2% (40–41 min) and 2% (41–51 min), increased linearly to 96% (51–52 min) and 96% (52–60 min). The total flow rate of the two pumps was 0.8 ml/min. MS scanning was performed in selected ion monitoring (SIM) mode that targeted specific [M+H]$^+$ ions for GDGTs.

For 5 samples around the transitional layer (L8, L9, L10, L11, U1), branched GDGTs (brGDGTs) were also measured according to a new method modified from
De Jonge et al. (2014) and Yang et al. (2015), on the HPLC/APCI-MS system at IEECAS. Separation of brGDGTs was obtained with two coupled Inertsil SIL-100A silica columns (each 250 mm × 4.6 mm, 3 μm; GL sciences Inc.) at 40 °C using isopropanol and n-hexane as elutes for pump A and pump B, respectively. The solvent gradient (for B) was: 0–85 min, decreased linearly from 97% to 95%; 85–89 min, decreased linearly from 95% to 10%; 89–108 min, held at 10% for cleaning; 108–112 min, increased linearly from 10% to 97%; 112–120 min, held at 97% for equilibration. The total flow rate of pump A and pump B was 0.6 ml/min. Selected ion monitoring (SIM) was used to target specific \([M+H]^+\) for brGDGTs. For each method, GDGTs were ionized in the APCI source at an interface temperature 350 °C, desolvation line 280 °C and heating block 250 °C, with the nebulizing gas and drying gas at 2.5 l/min and 5 l/min, respectively. Quantification of GDGTs was performed by integration of the peak area of \([M+H]^+\) ions in the extracted ion chromatogram, and comparison to that of the C_{46} internal standard. Compared with the traditional method, the new method enables the separation of 5-methyl and 6-methyl brGDGTs, and thus allows the calculation of new indices.

**Index calculations:** The carbon preference index (CPI, Bray and Evans, 1961) is a typical maturity index. It was calculated as in Hren et al. (2010):

\[
\text{CPI} = \frac{(n-C_{25} + n-C_{27} + n-C_{29} + n-C_{31} + n-C_{33})}{(n-C_{24} + n-C_{26} + n-C_{28} + n-C_{30} + n-C_{32})} + \frac{(n-C_{25} + n-C_{27} + n-C_{29} + n-C_{31} + n-C_{33})}{(n-C_{26} + n-C_{28} + n-C_{30} + n-C_{32} + n-C_{34})}
\]

(1)

The relative abundance of crenarchaeol to total isoprenoid GDGTs (isoGDGTs)
(%cren) index (Equation (2)) was calculated following Wang et al. (2014) to reconstruct lake-level variations:

\[
%\text{cren} = \frac{\text{cren}}{(\text{GDGT-0} + \text{GDGT-1} + \text{GDGT-2} + \text{GDGT-3} + \text{cren} + \text{cren isomer})}
\]

(Equation (2))

Early GDGT investigations showed that crenarchaeol is abundant in marine and large lakes while brGDGTs are predominant in terrestrial soil and peat. Therefore, Hopmans et al. (2004) defined the branched and isoprenoid tetraether (BIT) index (Equation (3)), which represents the relative abundance of the three major brGDGTs to crenarchaeol, as a proxy for estimating the relative amounts of terrestrial soil organic matter and aquatic organic matter in aquatic settings. However, recent studies have found that it is problematic when applied to trace terrestrial soil organic matter inputs (e.g. Fietz et al. 2012; Smith et al. 2012), due to the \textit{in situ} production of brGDGTs in aquatic systems (e.g. Tierney and Russell, 2009; Sinninghe Damsté et al., 2012; Loomis et al., 2014; Peterse et al., 2014; Hu et al., 2015) and the fact that the BIT index mainly depends on the aquatic production of crenarchaeol (Tierney et al., 2010; Fietz et al., 2011; Sinninghe Damsté et al., 2012; Smith et al., 2012; Buckles et al., 2015; Wang et al., 2016). On the other hand, because BIT index mainly depends on the aquatic production of crenarchaeol, which is strongly correlated with lake water depth (Tierney et al., 2010; Wang et al., 2014), variations in BIT index might reflect changes in lake water depth. Actually, significant negative relationships between BIT and lake water depth in 82 global lakes (Blaga et al., 2010) and 41 African lakes (Tierney et al., 2010) can be established across a full gradient of lake
environments (Fig. DR3; Wang et al., 2016). BIT has also been observed to trace water depth in both surface and downcore sediments of Lake Qinghai (Wang et al., 2016). Hence, it is also applied as a lake-level proxy in our analyses.

\[
\text{BIT} = \frac{(Ia + IIa + IIIa)}{(Ia + IIa + IIIa + cren)}
\]  

Currently, there are several brGDGT-based temperature and pH calibrations (reviewed in Schouten et al., 2013). Based upon a study of brGDGT distributions in over 130 globally distributed soils, Weijers et al. (2007) observed a significant correlation between soil pH and the cyclization ratio of branched tetraether (CBT) index (Equation (4)). Likewise, the methylation index of branched tetraether (MBT) index (Equation (5)) is positively correlated with the mean annual air temperature (MAT) and soil pH. Therefore, paleosoil pH and MAT can be quantified using CBT and the combination of MBT and CBT (MBT/CBT), respectively (Weijers et al., 2007). An extended survey of 278 globally distributed surface soils further confirmed that CBT relates best to soil pH, while the simplified form of MBT (i.e. MBT’) and CBT were shown to correlate with MAT (Peterse et al., 2012). In lacustrine sediments, however, the direct application of soil MBT/CBT (or MBT’/CBT) calibration might be problematic, because brGDGTs can be produced in situ in lakes, and their distribution can be quite different from that in catchment soils (e.g. Tierney and Russell, 2009; Wang et al., 2012; Loomis et al., 2014; Peterse et al., 2014; Hu et al., 2015). Therefore, a range of different lacustrine calibrations have been proposed (Tierney et al., 2010; Zink et al., 2010; Pearson et al., 2011; Sun et al., 2011; Loomis et al., 2012; Schoon et al., 2013; Foster et al., 2016). Amongst these lacustrine
brGDGT studies, Sun et al. (2011) provides the only calibration with global data while others are all regional. We thus have our pH and temperature reconstructed based on Sun et al. (2011) (Equation (6) and Equation (7)). It should be noted that the absolute temperature and pH values inferred from brGDGT indices should be viewed with caution due to calibration errors. For example, the calibration error for temperature estimate is 5°C, somewhat larger compared with other proxies such as those based on leaf or pollen analysis (Schouten et al., 2013). However, when the brGDGT temperature proxy is applied at a relatively small scale (i.e., comparing MAT estimates within a single record), the error becomes a systematic one which should be much lower (Peterse et al., 2011; Schouten et al., 2013). Hence, if brGDGTs were only used to reconstruct relative changes in MAT and pH, the potential errors should be small.

\[
\text{CBT} = -\log (I_b + I_{lb}) / (I_a + I_{la}) \quad (4)
\]

\[
\text{MBT} = (I_a + I_b + I_c) / (I_a + I_b + I_c + I_{la} + I_{lb} + I_{lc} + I_{IIIa} + I_{IIIb} + I_{IIIc}) \quad (5)
\]

\[
\text{pH} = 8.98 - 1.72 \times \text{CBT} \quad (6)
\]

\[
\text{MAT} = 3.949 - 5.593 \times \text{CBT} + 38.213 \times \text{MBT} \quad (7)
\]

The analytical reproducibility of the MBT and CBT indices is smaller than 0.01, resulting in an analytical error in temperature estimates of no more than 0.2 °C. Structures of the isoGDGTs and brGDGTs used for calculating %cren, BIT, and MBT/CBT are reviewed in Castañeda and Schouten (2011).

**Selection of GDGT methods:** Recently, De Jonge et al. (2013, 2014) identified a new set of 6-methyl brGDGT isomers which co-elute with 5-methyl brGDGTs in the
traditional analytical method that is commonly used so far. Further separation of
brGDGTs using an improved chromatographic method showed that the presence of
6-methyl brGDGTs may introduce scatter in the relationships between previous
brGDGT indices and MAT and pH in soils (De Jonge et al., 2014). Hence, new
indices which potentially provide more accurate soil pH and MAT estimates, i.e., the
CBT’ index (Equation (8)) which includes the 6-methyl brGDGTs, and the MAT_{mr}
index (Equation (9)) based on a multiple linear regression using the fractional
abundances of brGDGTs Ia, Ib, Ic and 5-methyl IIa, were proposed (De Jonge et al.,
2014).

\[
\text{CBT'} = \log \left[ \frac{(Ic + Ila' + IIb' + IIc' + IIIa' + IIIb' + IIIc')}{(Ia + IIa + IIIa)} \right] \quad (8)
\]

\[
\text{MAT}_{mr} = 7.17 + 17.1 \times [Ia] + 25.9 \times [Ib] + 34.4 \times [Ic] - 28.6 \times [IIa] \quad (9)
\]

Structures of brGDGTs used for calculating MAT_{mr} and CBT’ are described in De
Jonge et al. (2014).

\[
\text{pH} = 7.15 + 1.59 \times \text{CBT'} \quad (10)
\]

It should be noted, according to De Jonge et al. (2014), that the new indices
mainly showed significant improvement in arid soils, while in most other soils, the
reconstructed temperature and pH approximate those generated by the traditional
method. However, for lakes, until now there is no evidence that 6-methyl brGDGT
isomers could affect the temperature and pH reconstruction. Considering that the soil
calibration might not be appropriate for lakes (due to \textit{in situ} production) while new
lacustrine calibration is still lacking, the lacustrine calibration of Sun et al. (2011)
based on the traditional method are currently the most suitable one for the Clarkia
lacustrine deposits, at least for judging the trend and amplitude of temperature and pH variations.

To further test the robustness of using the traditional methods for brGDGT analysis (Hopmans et al., 2000; Schouten et al., 2007) and paleoclimate reconstruction (Weijers et al., 2007; Sun et al., 2011), we have measured brGDGTs for 5 of our samples around the transitional layer using the newly proposed method described in De Jonge et al. (2014). Applying the new indices and calibrations (Equations (8-10)), while the absolute values have slightly shifted, the reconstructed temperature and pH still exhibited negligible variation crossing the rapid shallowing event (Table DR2; Fig. DR4), in agreement with the results of the traditional method, excluding the possibility that the observed minimal variation in GDGT-derived MAT and pH is due to the use of a different GDGT method.

We also compared brGDGT-derived temperature with temperature estimates based on TEX_{86}. The TEX_{86} index (Schouten et al., 2002) also has the potential of reconstructing lake temperature (Powers et al., 2010), but its proper application is critically based on the premise that the four TEX_{86}-related GDGTs are derived predominantly from Thaumarchaeota living in the water column (Sinninghe Damsté et al., 2012). Methanotrophic archaea and methanogenic archaea, which could potentially generate some of the TEX_{86}-related isoGDGTs as Thaumarchaeota but lack the appropriate relationship with temperature, can affect TEX_{86} (Powers et al., 2010; Sinninghe Damsté et al., 2012). The imprint from methanotrophic archaea can be assessed by the so-called Methane Index (MI; Zhang et al., 2011), which varies
from 0 to 0.3 in normal marine conditions (Zhang et al., 2011). On the other hand, the abundance of GDGT-0 relative to crenarchaeol (%GDGT-0 = GDGT-0/[GDGT-0+crenarchaeol]*100) can be used to trace the activity of methanogenic archaea. %GDGT-0 higher than 67% (implying that GDGT-0/crenarchaeol > 2) may indicate significant influence of methanogenic archaea on GDGT distribution (Sinninghe Damsté et al., 2012). Using %GDGT-0 < 67 and MI < 0.3 as a criterion for the Clarkia lacustrine profile, the TEX$_{86}$ paleothermometer might be reliable only for samples in Unit 2d (Fig. DR5). Although temperature variations during the deposition of Unit 2d might be relatively small (ca. 4 °C and 3 °C based on TEX$_{86}$ and MBT/CBT, respectively), the trend of TEX$_{86}$-inferred lake temperature variation (according to the global lacustrine calibration of Castañeda and Schouten, 2011) in this unit is in general agreement with that derived from MBT/CBT (Fig. DR5), further suggesting that temperature variation estimated by MBT/CBT is generally valid for our samples.
**Figure DR1** Comparison of GDGT concentrations in the Miocene Clarkia lacustrine sediments vs. reported GDGT concentrations in surface sediments of modern lakes, including Qinghai Lake (Wang et al., 2012), Huguangyan Maar Lake (Hu et al., 2015), and South American lakes (Kaiser et al., 2015). Lower and upper sides of boxes indicate the 25th and 75th percentiles, respectively, while the horizontal lines inside boxes are the median values. The whiskers above and below the boxes indicate the maximum and minimum values, respectively.

**Figure DR2** Depth variations in the concentrations of brGDGTs and individual isoGDGTs.
Figure DR3 Relationships between the BIT index and water depth for 82 globally distributed lakes (Red dots, from Blaga et al., 2010) and 41 African lakes (Blue dots, from Tierney et al., 2010), modified from Wang et al. (2016). Although the global spread of lakes accompanies a full gradient of lake environments, a water depth of 18 m seems to be a threshold value for BIT values lower than 0.8.

Figure DR4 Variations of GDGT indices at the Clarkia P-33 section, including the water depth proxies (%cren and BIT), the reconstructed temperature (solid circle: according to Sun et al. (2011); open circle: according to De Jonge et al. (2014)), and the reconstructed lake water pH (solid circle: according to Sun et al. (2011); open circle: according to De Jonge et al. (2014)).
Figure DR5 Variations of GDGT indices at the Clarkia P-33 section, including the water depth proxies (\%cren and BIT), the TEX$_{86}$, MI, and \%GDGT-0 indices, and the reconstructed temperature based on MBT/CBT (green; according to Sun et al. (2011)) and reliable TEX$_{86}$ (orange; according to Castañeda and Schouten (2011)).
DATA REPOSITORY TABLES

Table DR1. GDGT and δD$_{\text{in-alkane}}$ data from Clarkia P-33 sequence. The gray shading indicates the transition unit (Unit 3).

| ID | Units | Height (cm) | GDGT-0 | GDGT-1 | GDGT-2 | GDGT-3 | cren. | cren' | IIla | IIlb | IIle | Ila | lb | le | TOC | %Cren | BIT | MAT | Lake pH | n-alkane δD (‰) |
|----|-------|-------------|--------|--------|--------|--------|-------|-------|------|------|------|-----|----|----|-----|------|------|-----|------|-----------------|------------------|
| U9 | 5c    | 290         | 613    | 79     | 44     | 26     | 35    | 3     | 944  | 30   | 22   | 1240| 155|25 | 991|160 | 38 | 4   | 0.99 | 11.8 | 7.5 | -217 | -218 | -217          |
| U8 | 5c    | 280         | 1003   | 105   | 72     | 39     | 46    | 5     | 1271| 31   | 25   | 1861|181|30 | 1435|233 |63 | 4   | 0.99 | 11.8 | 7.4 | -210 | -210 | -205          |
| U7 | 5c    | 270         | 1812   | 157   | 134    | 59     | 90    | 9     | 3450| 93   | 69   | 3707|349|56 | 2539|296 |77 | 4   | 0.99 | 8.9  | 7.3 | -211 | -214 | -211          |
| U6 | 5a    | 245         | 891    | 99    | 76     | 34     | 45    | 6     | 1353| 34   | 27   | 1553|133|26 | 1171|131 |35 | 4   | 0.99 | 9.7  | 7.2 | -215 | -216 | -215          |
| U5 | 5a    | 230         | 3745   | 303   | 229    | 87     | 148   | 12    | 5252|167  |108  | 5669|667|98 | 4292|507 |113 | 3   | 0.99 | 9.9  | 7.4 | -210 | -210 | -205          |
| U4 | 5a    | 215         | 2452   | 131   | 81     | 39     | 83    | 8     | 3019|93   | 74   | 3180|384|51 | 2483|289 |62 | 3   | 0.99 | 10   | 7.4 | -215 | -214 | -211          |
| U3 | 5a    | 200         | 1839   | 112   | 89     | 53     | 83    | 8     | 2359|70   | 42   | 2745|300|42 | 1894|245 |56 | 4   | 0.99 | 9.6  | 7.4 | -216 | -218 | -218          |
| U2 | 5a    | 185         | 1080   | 55    | 35     | 20     | 50    | 4     | 1378|76   | 49   | 1702|299|53 | 1307|177 |39 | 4   | 0.99 | 10.9 | 7.6 | -216 | -218 | -218          |
| U1 | 5a    | 170         | 1329   | 93    | 50     | 26     | 54    | 5     | 1553|69   | 30   | 1935|267|32 | 1552|186 |38 | 3.6 | 0.99 | 11   | 7.5 | -216 | -218 | -218          |
| L11| 3     | 110         | 2731   | 151   | 91     | 44     | 109   | 9     | 3429|152  |76   | 3721|518|64 | 3156|376 |80 | 3   | 0.99 | 10.9 | 7.5 | -221 | -219 | -222          |
| L10| 3     | 100         | 923    | 77    | 44     | 22     | 211   | 7     | 1050|50   | 18   | 1259|172|31 | 992 |123 |29 | 3.4 | 0.94 | 10.8 | 7.5 | -219 | -219 | -218          |
| L9 | 2d    | 90          | 4083   | 328   | 161    | 73     | 2504  | 39    | 3130|145  |66   | 3444|501|91 | 2660|338 |65 | 35  | 0.79 | 10.3 | 7.5 | -218 | -218 | -217          |
| L8 | 2d    | 80          | 2629   | 256   | 128    | 57     | 1716  | 28    | 1621|113  |38   | 1848|355|78 | 1431|213 |51 | 36  | 0.74 | 11   | 7.7 | -212 | -216 | -214          |
| L7 | 2d    | 70          | 2079   | 187   | 112    | 40     | 1375  | 20    | 1003|55   | 47   | 1193|223|38 | 997 |143 |32 | 36  | 0.7  | 11.6 | 7.6 | -216 | -216 | -216          |
| L6 | 2d    | 60          | 4864   | 397   | 197    | 79     | 3295  | 51    | 2876|141  |66   | 2983|487|65 | 2373|348 |67 | 37  | 0.71 | 10.8 | 7.6 | -217 | -217 | -217          |
| L5 | 2d    | 50          | 5011   | 430   | 163    | 82     | 3542  | 53    | 2592|126  |75   | 2669|506|73 | 2165|332 |79 | 38  | 0.68 | 11.1 | 7.7 | -217 | -217 | -217          |
| L4 | 2d    | 40          | 4599   | 425   | 178    | 77     | 3829  | 50    | 2297|144  |57   | 2405|526|83 | 1921|288 |76 | 42  | 0.63 | 11.1 | 7.7 | -217 | -217 | -217          |
| L3 | 2d    | 30          | 4985   | 463   | 170    | 78     | 4225  | 58    | 2403|119  |47   | 2612|448|82 | 1999|311 |133| 42  | 0.62 | 11   | 7.6 | -216 | -216 | -216          |
| L2 | 2d    | 20          | 3663   | 342   | 125    | 54     | 3408  | 43    | 1943|79   | 38   | 2146|273|50 | 1333|191 |45 | 45  | 0.61 | 8.9  | 7.5 | -213 | -216 | -209          |
| L1 | 2d    | 10          | 4425   | 366   | 128    | 57     | 4034  | 54    | 2844|94   | 48   | 2359|319|37 | 1485|193 |46 | 4.6 | 0.62 | 8   | 7.5 | -213 | -216 | -209          |
Table DR2. Fractional abundances of 16 brGDGTs and reconstructed temperature and pH for samples around the transitional layer analyzed according to De Jonge et al. (2014). IIIa” is a lake-specific brGDGT recently identified by Weber et al. (2015).

<table>
<thead>
<tr>
<th>ID</th>
<th>Fractional abundances</th>
<th>MATmr (°C)</th>
<th>pH</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>IIIa</td>
<td></td>
<td></td>
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<tr>
<td>L1</td>
<td>0.17</td>
<td>6.4</td>
<td>6.2</td>
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<td></td>
<td>IIIa”</td>
<td>0.02</td>
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<tr>
<td></td>
<td>IIIa’</td>
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<tr>
<td></td>
<td>IIIb</td>
<td>0.06</td>
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<tr>
<td></td>
<td>IIIb’</td>
<td>0.01</td>
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<tr>
<td></td>
<td>IIIc</td>
<td>0.01</td>
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<tr>
<td></td>
<td>IIIc’</td>
<td>0.01</td>
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<tr>
<td></td>
<td>IIa</td>
<td>0.17</td>
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<td></td>
<td>IIa’</td>
<td>0.02</td>
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<tr>
<td></td>
<td>IIb</td>
<td>0.06</td>
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<tr>
<td></td>
<td>IIb’</td>
<td>0.01</td>
<td></td>
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<td></td>
<td>IIc</td>
<td>0.01</td>
<td></td>
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<tr>
<td></td>
<td>IIc’</td>
<td>0.01</td>
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<tr>
<td></td>
<td>Ia</td>
<td>0.17</td>
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<td>Ib</td>
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<tr>
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