Biogeosciences Discuss.,
https://doi.org/10.5194/bg-2020-428-AC1, 2021

Biogeosciences Discussions

Interactive comment on "Development of global temperature and pH calibrations based on bacterial 3-hydroxy fatty acids in soils" *by* Pierre Véquaud et al.

Pierre Véquaud et al.

pierre.vequaud@upmc.fr

Received and published: 18 February 2021

We thank the anonymous reviewer for these comments. A detailed list of changes and arguments answering to the different comments is provided below.

Reviewers' comments:

Reviewer #1: Review

Summary - Véquaud and co-authors have compiled a large set of soils along elevation gradients in an attempt to determine global relationships of 3-OH FAs with MAAT and soil pH. They find that there is a global relationship with MAAT, but that relationships

Printer-friendly version

Discussion paper

are better on a local scale. They then use several statistical methods to quantify the relationships and to develop a temperature proxy based on 3-OH FAs. I appreciate the effort of the authors to compile this relatively large dataset and their attempt to assess the temperature and pH sensitivity of these compounds on a global scale. I do however have a few concerns and suggestions to further improve this work before I can recommend it for publication in Biogeosciences.

Author comment : We would like to thank the reviewer for his comments and for acknowledging the work made to evaluate the temperature and pH sensitivity of 3-OH FAs on a global scale. It should be highlighted that half of the 3-OH FA and brGDGT data presented in the manuscript are new (those corresponding to 4 altitudinal transects, i.e. Mt. Pollino, Italy; Mt. Shegyla, Tibet; Peruvian and Chilean Andes). Our new lipid data were combined with those previously published (Mt. Shennongjia, China, Yang et al., 2015 and Wang et al., 2016; Mt. Rungwe, Tanzania, Coffinet et al., 2017 and Huguet et al., 2019; Mt. Majella, Italy, Huguet et al., 2019; French Alps, Véquaud et al., 2021). Gathering these "old" and new data allowed establishing a large dataset which was used to evaluate the applicability of 3-OH FAs as MAAT and pH proxies in soils and to establish a comparison with the more established brGDGT proxies. Previous papers presenting brGDGT and 3-OH FA calibrations similarly rely on a combination of previously and newly acquired data (e.g. De Jonge et al., 2014; Naafs et al., 2017a; Huguet et al., 2019; Dearing Crampton-Flood et al., 2020).We also appreciate that the reviewer did not question the way the data were acquired, processed and interpreted.

Major comments: - BrGDGT data: Next to 3-OH FA data, the authors also present brGDGT data from the same samples. However, I fail to see the added value of the brGDGT data to this manuscript, and I thus suggest leaving this data out.

Author comment : We kindly disagree with the reviewer here. Indeed, to date, brGDGTs are the only organic proxies available for temperature and pH reconstruction in terrestrial settings. Therefore, as mentioned in the manuscript, the development of new molecular proxies, independent of and complementary to brGDGTs, is essential to improve the reliability of paleotemperature (and pH) reconstructions in such settings". 3-OH FAs could provide such a proxy. As a result, 3-OH FAs and brGDGTs have to be concomitantly analyzed to assess their reliability and complementarity as independent temperature and pH proxies. Such a comparison cannot be made if brGDGT data are not presented and cannot be used as "a reference proxy". The interest of brGDGT data in this manuscript will be further clarified in the revised version. It should also be noted that all the previous papers dealing with the influence of environmental parameters on 3-OH FA distribution in soils (Wang et al., 2016; Huguet et al., 2019; Véquaud et al., 2021) made a comparison between brGDGT-derived and 3-OH FA-derived proxies. Our approach is thus consistent with these previous papers.

a) the focus of the paper is on assessing the temperature and pH dependency of 3-OH FAs, which has nothing to do with brGDGTs.

Author comment : We agree with the reviewer that the main aim of this study is to evaluate the influence of pH and MAAT on 3-OH FA distribution in globally distributed topsoils. Nevertheless, it would be inappropriate not to compare these results with those derived from brGDGTs, the only other organic temperature/pH proxies terrestrial environments, as mentioned above. The comparison between brGDGT and 3-OH FA data is necessary, as it highlights the similarities and differences between these two independent families of molecules in terms of response to temperature and pH. This also shows the link between this study and previous ones dealing with the development of organic temperature/pH proxies in terrestrial settings. The different proxies and related studies should not be disconnected from each other.

b) most of the brGDGT datasets presented here are already published elsewhere.

Author comment : We kindly disagree with the reviewer, as only half of the brGDGT dataset is already published. The other half of the dataset, corresponding to 4 altitudinal transects (Mt. Pollino, Italy; Mt. Shegyla, Tibet; Peruvian and Chilean Andes), is presented here for the first time.

- In addition, the brGDGT data for two of the elevation transects (Rungwe and Shennongjia) are based on ‘old’ chromatography methods that do not separate the 5- and 6-methyl brGDGT isomers. Note that these datasets should not be directly compared with ‘new’ brGDGT data for the other transects, as MAATs and pH are derived based on different equations. The ‘old’ MBT and CBT indices both contain compounds that appear to have a 6-methyl isomer (e.g. IIa and IIIa in the MBT index, and IIa and IIb in the CBT index). This makes it impossible to determine whether a relative change in the peak area of one of these compounds is driven by the 5- or by the 6-methyl isomer. Especially in the case of MBT this is problematic, as the occurrence of 6-methyl brGDGTs is linked to changes in pH and not MAAT (De Jonge et al., 2014). The authors may be unaware, but ‘new’ brGDGT data for Mt. Shennongjia has been published by Yang et al., 2015, who, in fact, state that 6-methyl brGDGTs significantly affect the performance of the MBT’ in this transect, proving my point that the use of ‘new’ data is important (if at all, in case of this manuscript).

Author comment : We totally agree with the reviewer on the importance of separating 5- and 6-methyl brGDGT isomers and never said the opposite in our paper. The new data presented in this study were all obtained using two silica columns, allowing the separation of these isomers. Similarly, previously published brGDGT data from the French Alps (Véquaud et al., 2021) and Mt. Majella (Huguet et al., 2019) were also acquired with this new methodology. Regarding Mt. Shennongjia, we agree with the reviewer that 5- and 6-methyl brGDGTs were indeed separated in the Organic Geochemistry paper published by Yang et al. (2015). However, the relative abundances of the individual 5- and 6-methyl brGDGTs were not directly provided in this paper, which prevented us to use them. Following up the review, the authors kindly sent us these data upon request. These abundances and the values of MBT’5Me index can now be used in our paper. This point will be clarified in the revised manuscript. On the whole, data from 7 out of 8 transects investigated in this study were obtained using the “new” chromatography method allowing the separation of 5- and 6-methyl brGDGTs. All these data can be directly compared and exploited. This will be clearly mentioned in the revised manuscript. Regarding the data from Mt. Rungwe, they were obtained using the "old" chromatography method relying on a cyano column. As 5- and 6-methyl brGDGTs were not separated, this dataset cannot be directly compared with the 7 others. Nevertheless, the data for the 8 transects with the old brGDGT separation method will be presented as supplementary data in the revised version of the manuscript. These results show the same trends with and without isomer separation.

- Ecology of 3-OH FA producers: There are several points in the manuscript where the authors state that a better understanding of the adaptation mechanisms of 3-OH FA producing organisms to changing environmental conditions may improve the proxies (e.g. L484), or that the use of (a) subset(s) of 3-OH FAs could results in better relations with MAAT or pH (as suggested for the RIAN-pH relationship). I feel that there is a missed opportunity here and improvements should be made in a revised version. If it is known that 3-OH FAs are produced by Gram negative bacteria, what can we tell about their occurrence, response to environmental change, etc? Or is this group simply too big to say anything sensible?

Author comment : 3-OH FAs are produced by Gram-negative bacteria which, as suspected by the reviewer, are a highly diverse, non-monophyletic and ubiquitous group of microorganisms represented by numerous genera (Lecointre and Guyader, 2006). This explains the large genetic and biochemical differences between the various Gram-negative bacteria. The numerous genera of Gram-negative bacteria are characterized by highly diverse lipid profiles, with different relative abundances of the C10-C18 3-OH FAs, and by the fact that all the homologues are not biosynthesized by all the strains (Wilkinson et al., 1988). Thus, the 3-OH FA lipid distribution in soils is highly dependent on the diversity of Gram-negative bacterial species (Parker et al., 1982; Bhat and Carlson, 1992; Zelles, 1999), which may vary with altitude (Margesin et al., 2009; Siles and Margesin, 2016). Considering these different facts, it is difficult to draw out a general hypothesis on the response of Gram-negative bacteria and their associated lipids to environmental changes. A multiplicity of environmental parameters, including

MAAT and pH, may have an influence on 3-OH FA lipid distribution. The latter can reflect changes in the diversity of bacteria communities (e.g. Siles and Margesin, 2016) and/or adaptation of a constant community.

- Proxy model development From the brGDGT and other biomarker proxy studies we have learned that many of the transfer functions based on linear regressions suffer from regression dilution (e.g. Tierney and Tingley, 2014; Naafs et al., 2017; Dearing-Crampton-Flood et al., 2020). I miss an assessment of this aspect for the 3-OH FA proxies in this manuscript, which are all based on methods that involve linear regressions.

Author comment : We agree with the reviewer that a weak point of all methods based on regression methods is that they suffer from the phenomenon of regression dilution. That is why proposing alternative models that are not based on linear regression methods, such as those proposed in this study (random forest and k-NN algorithms), represent a major advantage. This aspect will be clearly mentioned in the revised manuscript and better assessed.

-I would also like to point out that there is a general move towards using Bayesian statistics to derive proxies. This approach will allow you to treat your biomarker-based index as dependent variable in the calibration model whilst accounting for possible errors in the measurement of both MAAT and your biomarker index (see the explanation in the introduction of Dearing Crampton-Flood et al., 2020). I encourage the authors to look into this method and consider its use for their purpose.

Author comment :Several methods were recently used to derive calibrations from organic proxies, such as multivariate regression (Russell et al., 2018), Deming regression (Naafs et al., 2017) , Bayesian linear regressions models (Tierney and Tingley, 2014; Dearing Crampton-Flood et al., 2020) or machine-learning models (Dunkley Jones et al., 2020). None of these methods excludes or prohibits the use of the others. Independent models should be used for the development of environmental calibrations, as each of them has its own advantages and drawbacks. The different models have to be seen as complementary. As mentioned by the reviewer, Bayesian statistics were recently used to develop new calibration models, e.g. with brGDGTs (Dearing Crampton-Flood et al., 2020). The robustness of the Bayesian models relies on the fact that they consider a given index (for example, the MBT'5Me for brGDGTs) as the variable dependent on environmental parameters, in contrast with models based on linear regressions. This is realistic, as lipids are produced in response to the variations of environmental parameters. This model also avoids regression dilution phenomena, as mentioned by the reviewer. Nevertheless, the Bayesian method is always restricted to the use of an index, which allows the reconstruction of a given environmental parameter (for example temperature). This represents a limitation, as the relative distribution of bacterial lipids can be concomitantly influenced by several environmental parameters (e.g. Véquaud et al., 2021). In contrast, using bacterial relative abundances rather than a single index in models appears less restrictive, and more representative of the environmental complexity. The different models (multiple regression, k-NN method, Random Forest) presented in this paper allow overcoming the limitations related to the use of a single index, as they take into account the whole suite of bacterial lipids (here C10-C18 3-OH FAs) to estimate MAAT and pH values. In addition, the Bayesian model is parametric and it only takes into account linear relationships. Conversely, the k-NN and Random Forest models used in this study are non-parametric and can take into account non-linear environmental influences, in line with the intrinsic complexity of the environmental settings. This helps in improving the reliability of the models. Moreover, the models based on machine learning algorithms are built on a proportion of the total dataset (randomly defined) and then tested on the rest of the dataset, considered as independent. Such an approach improves the robustness of the models. As the Bayesian model, the k-NN and random forests are not based on linear regressions, thus avoiding the phenomenon of regression dilution. In conclusion, we chose the k-NN and random forest models in the present study, as they present major advantages for the development of robust calibrations between bacterial lipid distribution and environmental parameters, as explained above. Such a choice will be better justified and discussed in the revised manuscript. Once again, this does not exclude the use of other independent and complementary models, such as those based on Bayesian statistics, but this is beyond the scope of the present study.

- Application of the 3-OH FA proxies The authors have chosen a stalagmite as test archive for their proxy. but I really do not think that a speleothem is a suitable archive to test proxies that are based on the occurrence and behavior of 3-OH FAs in soils. Speleothems and soils are completely different environments, and it is no way guaranteed, let alone tested that the sources of 3-OH FAs in both environments are the same, let alone their relationship with temperature and/or pH. I would either leave this example out, or find another (soil!) archive to test their proxies.

Author comment : Testing the performance and validity of the proposed global models on an existing archive is essential, as the calibration models are developed from modern samples to then provide robust and reliable paleoreconstructions. Most of the recent studies proposing new global or local MAAT calibrations, based on either brGDGTs or 3-OH FAs, adopted this approach and applied their models to a well-constrained archive to assess its robustness and accuracy (e.g. Naafs et al., 2017; Dearing Crampton-Flood et al., 2020; Wang et al., 2020; Yang et al., 2020). As a result, we developed MAAT calibrations from 3-OH FA distribution in soils using machine learning models (k-NN and random forest algorithms) and then tested and compared these calibrations using a speleothem archive. We agree with the reviewer that a soil archive would have better fitted to test our new calibrations and that soils and speleothems are different terrestrial settings. Nevertheless, the validation of the terrestrial models we propose requires using a well-known archive, for which paleoclimatic and paleoenvironmental data are available. This allows constraining the climatic/environmental conditions at the time of the reconstruction based on a multi-proxy approach. So far, the only 3-OH FA based paleorecord available in the literature is the Chinese speleothem previously investigated by Wang et al. (2018), which was the object of previous paleostudies, thus providing a context for the interpretation of the MAAT data. Moreover, Wang et al. (2018) suggested that the 3-OH FAs in the investigated speleothem are largely derived from the overlying soils based on the "broad similarity of 3-OH FA distributions in the overlying soils and stalagmites" as well as "site-specfic analyses of bacterial diversity and transport pathways". Thus, using 3-OH FA-based soil calibrations to reconstruct MAAT/pH from this speleothem is not so illogical. By the way, a local Chinese MAAT calibration obtained after the analysis of 3-OH FAs in 26 soil samples (Wang et al., 2016) was previously applied to this record. In the present study, we compare the MAAT estimates provided by our global soil calibrations with those previously obtained using the local calibration by Wang et al. (2016). In conclusion, it seems reasonable to us to test our new models on a terrestrial archive (even though this is not a soil) to show their potential and limits, as the concrete goal of such calibrations is to be used in the framework of paleoenvironmental studies. Such a choice will be better justified in the revised version of the manuscript to avoid any confusion in the mind of the reader.

- Data compilation I notice that the authors have included one dataset that is still under review in Organic Geochemistry (Véquaud et al.,). In case this manuscript is accepted first (actually, the data is already published online as part of this discussion paper), is there any novelty left for the manuscript in OG? Aren't you shooting yourself in the foot here?

Author comment : We thank the reviewer for this concern. However, there is no problem since the OG manuscript is in press (Véquaud et al., 2021) and available online (https://doi.org/10.1016/j.orggeochem.2021.104194). The OG paper aimed to investigate in detail the influence of environmental parameters on 3-OH FA distribution in soils from the French Alps. The present paper notably uses the data from the OG paper to create a large dataset based on soils from all over the world.

Minor comments:

Printer-friendly version

Discussion paper

L70: the use of Eglinton and Eglinton as a reference to proxies based on membrane lipids is technically not incorrect, but it seems more appropriate to use e.g. Schouten et al., 2002, Weijers et al., 2007 ('they were first'), or the re-view paper of Schouten et al., 2013.

Author comment : This will be corrected in the revised version of the manuscript.

L79: For aquatic environments, references to Peterse et al., 2009 (marine brGDGTs) and Tierney and Russell, 2009 and Sinninghe Damsté et al., 2009 (lacustrine brGDGTs) are better suited ('they were first').

Author comment : These references will be added in the revised version of this paper.

L98: explain what RAN15 and RAN17 stand for prior to using the abbreviation.

Author comment : This will be corrected.

L109: re-place calibration by relation L112: explain RIAN prior to using the abbreviation.

Author comment : This will be amended.

L130: replace 'collected along globally distributed' by 'determined in several elevation tran-sects'

Author comment : This sentence will be corrected following this comment.

L134: This sentence is not really grammatically correct. Rewrite to somethinglike 'even though brGDGT-based MAAT and pH reconstructions still have a relatively large uncertainty, they can serve as a reference to test the temperature dependency of 3OH FAs analyzed in the same dataset.'

Author comment : This sentence will be corrected as suggested.

L137: use either 'the 3OH FA distribution'or '3OH FA distributions'.

Author comment : This will be corrected.

L177: what is a 'fir'?

Author comment : Abies forrestii is a species of conifer in the family of Pinaceae, commonly referred as Forrest's fir. This sentence will be clarified in the revised version.

L230: can you add the compound that was used as an internal standard?

Author comment : The internal standard was a deuterated and methylated 3-OH fatty acid, the 3-hydroxytetradecanoic acid, 2,2,3,4,4-d5 (Sigma-Aldrich, France). This will be specified in the revised version of the paper.

L274: Is there a reason why the latest definition of the CBT' index by De Jonge et al., 2014 was not used (their Eq. 10)? This index takes the separation of 5- and 6-methyl isomers into account and also has a lower RMSEcompared to the one of Peterse et al., 2012 that is based on data generated with the'old' chromatography method. If not, I would recommend using the CBT' index.

Author comment : As suggested by the reviewer, the CBT' will be used in this manuscript instead of the CBT index. Nevertheless, the interpretations and conclusions from the CBT' remain the same as with the CBT, as the values of the two indices are similar.

L397: replace inertia by variance (inertia means the tendency to remain unchanged, which isnot what you mean here, I presume)

Author comment : This will be corrected.

L400: how reliable is 'location' as a factor influencing 3OH FAs? I don't really think that microorganisms would take their coordinates intoaccount when they synthesize 3OH FAs. Instead, I suspect that location represents anindirect parameter that integrates the local environmental conditions at each site. Thus, 3OH FAs are more likely linked to temperature, precipitation, vegetation, pH, whateveron the first PC, so I suggest re-running the PCA without taking location into account.

Author comment : We think there is a misunderstanding here. In fact, the PCAs were performed using the fractional abundances of the bacterial lipids (3-OH FAs and brGDGTs) in the total dataset, without taking the location into account. Nevertheless, it is possible to statistically qualify which variables best explain the distribution of the samples in the PCA. It clearly appears that the samples are located in the PCA based on to their location, which reflects the contrasting environmental conditions influencing the 3-OH FA and brGDGT source organisms at each site. This point will be clarified in the revised version of this manuscript.

L457-459: this sentence seems to be missing words?

Author comment : This sentence will be corrected as follows: "The distribution of 3-OH FAs varies greatly among Gram-negative bacterial species (Bhat and Carlson, 1992), which may account for significant variability in RIAN values among soils within a given transect".

L459: is the lack of a relationbetween the RIAN and pH caused by the use of a linear model, or by the relativelysmall range of soil pH of this dataset? How can you tell? And would another modelbe better suitable to capture this relation? If so, which kind of model?

Author comment : In our global dataset, pH values range between 3 and 8. This cannot be considered as a small range of variation. Our hypothesis is that more complex models (non-parametric and non-linear models, e.g. Random forest, k-NN method) take into account the non-linear influences of environmental parameters on lipid distribution and can be more suitable to specifically explain the relationship between 3-OH FA distribution and pH values. This point will be clarified in the revised version of the manuscript.

L467: Please refer to and compare with the newer calibration studies. Several have been publishedsince 2012, but at least use De Jonge et al., 2014 that includes the 5- and 6-methylisomers.

Printer-friendly version

Discussion paper

Author comment : As previously suggested, the CBT' index will be used instead of the CBT and will allow a direct comparison with the newer calibration studies (e.g. De Jonge et al., 2014). This reference and comparison will be added in the revised version of the manuscript.

L490: replace similarly by also L492 (here and elsewhere in the ms): replace'prediction interval' by 'confidence interval'.

Author comment :This will be corrected.

L542ff: How does the MBT'5me relationwith MAAT from this study compare to the one in the global surface soil dataset? Doesit have the same slope and intercept?

Author comment : The relationship between the MBT'5Me and the MAAT obtained in this study (MAAT = 24.5 × MBT'5Me -4.78) follows a similar trend as the global calibration proposed by De Jonge et al. 2014 (MAAT = 31.45 × MBT'5Me - 8.57). In the next version of this manuscript, a direct statistical comparison between these two calibrations will be proposed.

General: Replace Damsté by Sinninghe Damsté Author comment : This will be made.

Figures 1 and 2: I'm not sure how useful it is to show the relative distributions of 3OH-FAs and brGDGTs, especially since every site represents an elevation gradient along which a large variation in temperature (and thus biomarker composition) is expected.Instead, display the proxy values with elevation (or completely delete them, as the proxies are already plotted against pH and MAAT in Figs 4-6).

Author comment : These figures showing the relative distributions of 3OH-FAs and brGDGTs are useful to understand the natural variability of these compounds along the different transects. This comprehension is necessary to understand the PCAs calculated with the fractional abundances of 3-OH FAs and brGDGTs.

Figures 4 and 5 and 6. Can you add the regressions, or at least the regression coefficient (R2) of eachsignificant regression to the panels?

Figure 9: The y-axis of panel a does not have atitle

Author comment : These figures will be modified and corrected according to these comments.âĂČ

References Bhat, U.R., Carlson, R.W., 1992. A new method for the analysis of amide-linked hydroxy fatty acids in lipid-As from gram-negative bacteria. Glycobiology 2, 535–539.

Coffinet, S., Huguet, A., Pedentchouk, N., Bergonzini, L., Omuombo, C., Williamson, D., Anquetil, C., Jones, M., Majule, A., Wagner, T. and Derenne, S., 2017: Evaluation of branched GDGTs and leaf wax n-alkane δ2H as (paleo) environmental proxies in East Africa, Geochimica et Cosmochimica Acta, 198, 182–193, doi:10.1016/j.gca.2016.11.020.

De Jonge, C., Hopmans, E.C., Zell, C.I., Kim, J.-H., Schouten, S., Sinninghe Damsté, J.S., 2014. Occurrence and abundance of 6-methyl branched glycerol dialkyl glycerol tetraethers in soils: Implications for palaeoclimate reconstruction. Geochimica et Cosmochimica Acta 141, 97–112.

Dearing Crampton-Flood, E., Tierney, J.E., Peterse, F., Kirkels, F.M.S.A., Sinninghe Damsté, J.S., 2020. BayMBT: A Bayesian calibration model for branched glycerol dialkyl glycerol tetraethers in soils and peats. Geochimica et Cosmochimica Acta 268, 142–159.

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, 2599–2617.

Huguet, A., Coffinet, S., Roussel, A., Gayraud, F., Anquetil, C., Bergonzini, L., Bonanomi, G., Williamson, D., Majule, A., Derenne, S., 2019. Evaluation of 3-hydroxy fatty acids as a pH and temperature proxy in soils from temperate and tropical altitudinal gradients. Organic Geochemistry 129, 1–13.

Lecointre G. and Guyader H. L. 2006. The Tree of Life: A Phylogenetic Classification., Harvard 925 University Press

Margesin, R., Jud, M., Tscherko, D., Schinner, F., 2009. Microbial communities and activities in alpine and subalpine soils: Communities and activities in alpine and subalpine soils. FEMS Microbiology Ecology 67, 208–218.

Naafs, B.D.A., Gallego-Sala, A.V., Inglis, G.N., Pancost, R.D., 2017a. Refining the global branched glycerol dialkyl glycerol tetraether (brGDGT) soil temperature calibration. Organic Geochemistry 106, 48–56.

Naafs, B.D.A., Inglis, G.N., Zheng, Y., Amesbury, M.J., Biester, H., Bindler, R., Blewett, J., Burrows, M. A., del Castillo Torres, D., Chambers, F.M., Cohen, A.D., Evershed, R.P., Feakins, S.J., Gałka, M., Gallego-Sala, A., Gandois, L., Gray, D.M., Hatcher, P.G., Honorio Coronado, E.N., Hughes, P.D.M., Huguet, A., Könönen, M., Laggoun-Défarge, F., Lähteenoja, O., Lamentowicz, M., Marchant, R., McClymont, E., Pontevedra-Pombal, X., Ponton, C., Pourmand, A., Rizzuti, A.M., Rochefort, L., Schellekens, J., De Vleeschouwer, F., Pancost, R.D., 2017b. Introducing global peat-specific temperature and pH calibrations based on brGDGT bacterial lipids. Geochimica et Cosmochimica Acta 208, 285–301.

Parker, J.H., Smith, G.A., Fredrickson, H.L., Vestal, J.R., White, D.C., 1982. Sensitive assay, based on 959 hydroxy fatty acids from lipopolysaccharide lipid A, from Gram negative bacteria in sediments. 960 Applied and Environmental Microbiology 44.

Russell, J.M., Hopmans, E.C., Loomis, S.E., Liang, J., Sinninghe Damsté, J.S., 2018. Distributions of 5- and 6-methyl branched glycerol dialkyl glycerol tetraethers (brGDGTs) in East African lake sediment: Effects of temperature, pH, and new lacustrine paleotemperature calibrations. Organic Geochemistry 117, 56–69. Siles, J.A., Margesin, R., 2016. Abundance and Diversity of Bacterial, Archaeal, and Fungal Communities Along an Altitudinal Gradient in Alpine Forest Soils: What Are the Driving Factors? Microbial Ecology 72, 207–220.

Tierney, J.E., Tingley, M.P., 2014. A Bayesian, spatially-varying calibration model for the TEX86 proxy. Geochimica et Cosmochimica Acta 127, 83–106.

Véquaud, P., Derenne, S., Anquetil, C., Collin, S., Poulenard, J., Sabatier, P., Huguet, A., 2021. Influence of environmental parameters on the distribution of bacterial lipids in soils from the French Alps: Implications for paleo-reconstructions. Organic Geochemistry 104194.

Wang, C., Bendle, J., Yang, Y., Yang, H., Sun, H., Huang, J. and Xie, S., 2016: Impacts of pH and temperature on soil bacterial 3-hydroxy fatty acids: Development of novel terrestrial proxies, Organic Geochemistry, 94, 21–31, doi:10.1016/j.orggeochem.2016.01.010.

Wang, C., Bendle, J.A., Zhang, H., Yang, Y., Liu, D., Huang, J., Cui, J., Xie, S., 2018. Holocene temperature and hydrological changes reconstructed by bacterial 3-hydroxy fatty acids in a stalagmite from central China. Quaternary Science Reviews 192, 97–105.

Wang, H., An, Z., Lu, H., Zhao, Z., Liu, W., 2020. Calibrating bacterial tetraether distributions towards in situ soil temperature and application to a loess-paleosol sequence. Quaternary Science Reviews 231, 106172.

Wilkinson, S.G. 1988 Gram-negative bacteria. In: Ratledge C., Wilkinson S.G. (Eds), Microbial Lipids, 1063 vol. 1. Academic Press, New York, pp. 199-488.

Yang, H., Lü, X., Ding, W., Lei, Y., Dang, X. and Xie, S., 2015: The 6-methyl branched tetraethers significantly affect the performance of the methylation index (MBTâĂš) in soils from an altitudinal transect at Mount Shennongjia, Organic Geochemistry, 82, 42–53, doi:10.1016/j.orggeochem.2015.02.003.

Yang, Y., Wang, C., Bendle, J.A., Yu, X., Gao, C., Lü, X., Ruan, X., Wang, R., Xie, S., 2020. A new sea surface temperature proxy based on bacterial 3-hydroxy fatty acids. Organic Geochemistry 141, 103975.

Zelles, L., 1999. Fatty acid patterns of phospholipids and lipopolysaccharides in the characterisation of microbial communities in soil: a review. Biology and Fertility of Soils 29, 111–129.

Interactive comment on Biogeosciences Discuss., https://doi.org/10.5194/bg-2020-428, 2020.