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

Anonymous Referee #1

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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 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.

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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. Especially given the facts that 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, and b) most of the brGDGT datasets presented here are already published elsewhere. 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).

- 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

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their occurrence, response to environmental change, etc? Or is this group simply too big to say anything sensible?

- 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. 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.

- Application of the 3-OH FA proxies The authors have chosen a stalagmite as test archive for their proxy. It may be the only 3-OH FA-based paleorecord in the literature so far, 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.

- 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?

Minor comments: 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 review paper of Schouten et al., 2013. 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'). L98: explain what RAN15 and RAN17 stand for prior to using the abbreviation. L109: replace calibration by relation L112: explain RIAN prior to using the abbreviation. L130: replace 'collected along globally distributed' by 'determined in several elevation transects' L134: This sentence is not really grammatically correct. Rewrite to something like '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.' L137: use either 'the 3OH FA distribution' or '3OH FA distributions'. L177: what is a 'fir'? L230: can you add the compound that was used as an internal standard? 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 RMSE compared 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. L397: replace inertia by variance (inertia means the tendency to remain unchanged, which is not what you mean here, I presume) L400: how reliable is 'location' as a factor influencing 3OH FAs? I don't really think that microorganisms would take their coordinates into account when they synthesize 3OH FAs. Instead, I suspect that location represents an indirect parameter that integrates the local environmental conditions at each site. Thus, 3OH FAs are more likely linked to temperature, precipitation, vegetation, pH, whatever on the first PC, so I suggest re-running the PCA without taking location into account. L457-459: this sentence seems to be missing words? L459: is the lack of a relation between the RIAN and pH caused by the use of a linear model, or by the relatively small range of soil pH of this dataset? How can you tell? And would another model be better suitable to capture this relation? If so, which kind of model? L467: Please

refer to and compare with the newer calibration studies. Several have been published since 2012, but at least use De Jonge et al., 2014 that includes the 5- and 6-methyl isomers. L490: replace similarly by also L492 (here and elsewhere in the ms): replace 'prediction interval' by 'confidence interval'. L542ff: How does the MBT'5me relation with MAAT from this study compare to the one in the global surface soil dataset? Does it have the same slope and intercept?

General: Replace Damsté by Sinninghe Damsté

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). Figures 4 and 5 and 6. Can you add the regressions, or at least the regression coefficient (R2) of each significant regression to the panels? Figure 9: The y-axis of panel a does not have a title.

References: Dearing Crampton-Flood et al., 2020 GCA 268, 142-159 De Jonge et al., 2014 GCA 141, 97-112 Naafs et al., 2017 Org geochem 106, 48-56. Peterse et al., 2009 Org Geochem 40, 692-699. Peterse et al., 2012 GCA 96, 215-229. Schouten et al., 2002 EPSL 204, 265-274. Schouten et al., 2013 Org Geochem 54, 19-61. Sinninghe Damsté et al., 2009 GCA 73, 4232-4249. Tierney and Tingley, 2014 GCA 127, 83-106 Tierney and Russell, 2009 Org Geochem 40, 1032-1036 Weijers et al., 2007 GCA 71, 703-713 Yang et al., 2015 Org Geochem 82, 42-53.

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