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Interactive comment on "Climate reconstructions based on GDGTs and pollen surface datasets from Mongolia and Siberia: Calibrations and applicability to extremely dry and cold environments" *by* Lucas Dugerdil et al.

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Responses to the comments of Reviewer 2 (David Naafs)

General comments:

In this manuscript Dugerdil and co-authors determine pollen and GDGT distributions in a set of surface samples (mineral soil, moss, and lake sediment) from Mongolia and

Siberia to establish novel (local) climatic calibrations (precipitation and temperature). I am not an expert in pollen and therefore focus my review on the GDGT-part of the manuscript. I hope other reviewers can comment on the pollen methods and results. I congratulate the authors with writing a manuscript that reads well and with references that are up to date. The figures are also well made. I especially like figure 7 that manages to clearly display a lot of information (but check if it is suitable for colourblind people?). I think this is an elegant dataset from a poorly studied region that is valuable to the paleoclimate, pollen, and GDGT community.

However, I have a number of comments that need to be addressed before publication.
- Firstly, the foundation for the calibrations: the instrumental data. Given the few weather stations in the region (line 169), what is the error on the instrumental data (temperature and precipitation) for the calibrations? For example, for temperature is it 1 or 5 C or more? How confident are we that we know the temperature that the samples experienced? This error should be taken into account into the calibrations and discussed properly.

Response and applied changes: The climate data originate from the WorldClim2 database. The error on the climatic parameters is linked to elevation and distance to stations. Because these two sets of information, it should possible to provide uncertainties. Such a modeling could however be the topic of a whole article per se, we therefore based our analyses on the errors proposed by Fick and Hijmans (2017) for the Arid Central Asian Area. The interpolation model used f(x,y,z, coast, sat) in this area give a R-squared = 0.994 and RMSE = 1.344. This error was established on a large geographical area, for which elevation and isolation (average distance between two meteorological stations) are basically similar to the Mongolian plateau. Similar reasoning was followed for MAP : R^2 = 0.894 and RMSE = 23.241 mm.yr-1. We mentioned these errors in the manuscript (Paragraph 5.4 followed, L.

419) and added the following sentence: "*According to the authors, the interpolation model used in the Central Arid Area (which includes our study area) gives R^2 = 0.99 and RMSE = 1.3 C for MAAT and R^2 = 0.89 and RMSE = 23 $mm.yr^{-1}$ for MAP. Whenever the Siberian-Mongolian calibrations are used for palaeoclimatic reconstructions, the RMSE of the climate parameters have to be added to the RMSE model.*"

Also, the discussion focuses on mean annual temperature, but did you explore warm season temperatures? Especially for the cold regions this might improve the calibration. If not, this is also interesting and should be discussed.

Response: For pollen transfer functions, the Mean Temperature of the Warm Period (MTWA) or spring temperatures seem to better fit than the MAAT on siberian-mongolian clipped databases. Similarly, for br-GDGTs, MR-models have also been calculated with MTWA and summer temperatures. These models do not however perform significatively better than those with MAAT. For example, the $MTWA_{mr6}$ (6 parameters) presents R^2 = 0.63, RMSE = 1.53C and AIC = 178. As summer temperatures are concerned, $MTWA_{mr6}$ displays the exact same values (probably because MTWA and Tsum are roughly spreading on the same time-laps). Similarly, MTWA do not perform significantly better than MAAT mr-models. Although this lack of seasonality is quite surprising (because of the permafrost impact on bacterial communities), this result is consistent with the Chinese sites not showing any seasonal bias (Lei et al., 2016).

Applied changes : At the end of the second part of the 5.4 paragraph (L. 445) : "*Even if GDGTs seem to react to summer temperature, (Wang et al., 2016; Kusch et al., 2019) the mr-models are not significantly improving the calibration than the* $MAAT_{mr}$ *ones. For instance, the best* $Tsum_{mr}$ *is selected by its AIC,* $Tsum_{mr6}$ *using 6 br-GDGTs fractional abundance displays R^2 = 0.63 and RMSE = 1.53 C. The lack of seasonality,*

expected in such cold areas, is consistent with temperate Chinese sites (Lei et al., 2016)."

-I find it odd that lake sediment samples are combined with mineral soil and moss samples. Does that mean the new calibrations can be applied to both archives? We know that the brGDGT distribution in lakes differs with that in soils (compare mineral soil brGDGT data versus temperature with that of lakes). I suggest the authors split the lake and soil data into different calibrations. Does that improve the correlation for for example MBT5me'? Also compare the lake samples with the recent lake calibrations (Russell et al., 2018). In addition, for lake sediments I expect no correlation between brGDGT distribution and local precipitation (as they are mainly formed in the water column), was this taken into account to obtain the MAP calibrations?

Response: This concern is important and was similarly raised by Referee 1 (see the response and the associated changes in the answer to Referee 1).

-But then there is the more fundamental problem: Using R^2 values and other statistical methods to select the best calibration. I appreciate that the authors take overparametrization into account (section 5.1) but I think a major problem with their approach is that we end up with complex calibrations that include compounds that are not very abundant (e.g. brGDGT-IIIa' and -IIIc). Minor changes in the abundance of these minor compounds (or even slightly different ways of integrating the minor peaks) can have a major impact on the resulting temperature. I think it would be valuable to only consider compounds that have a certain relative abundance, like > 5-10 %. How would this impact the selected calibrations? In addition, this way we lose any physical basis for the proxy. The original MBT proxy reflects a decrease in degree of methylation with increasing temperature and this has a physical meaning for membrane properties and hence provides confidence that this is a true signal and not a random empirical observation. But what is the impact on a bacterial membrane if it is has a few percent more of brGDGT-IIIb'? What is the physical basis of these new calibrations and hence are we confident that these are real temperature relationships? This aspect needs a thorough consideration and discussion.

Response and applied changes: We acknowledge this comment, but we wish to raise several related issues:

- First, the "minor compounds" are not identical depending on the setting. For example, IIIa' and IIIc are respectively the 4th and the 9th compound by relative abundances over the 15 compounds. Furthermore, the compound distributions in the Siberian-Mongolian area differ from the global peatland and soil database (Figure X). In global datasets, the relative abundances are damped because the over representation of Ia (45 to 75 % in peat samples) and IIa (15 to 40 % in peat samples). In mongolian soils, these two compounds are less abundant, 10 to 20 % and 5 to 15%, respectively (Figure X).
- Applied changes: Paragraph 4.2.3 : "Even the models including minor compounds ([br]i<5%) have been studied. In the NMSDB brGDGT fractional abundances are indeed more fairly distributed than in the global database, where some compounds overlaps the others (Annex Figure B2.C and D)"
- Furthermore, when compound cumulative means are considered (Annex fig. B2.D), the curve issued from the Mongolian dataset is flatter than the global peat and soil ones. The impact of minor compounds finally appear more important than in other studies. This is especially the case for some compounds, not abundant in the global context but more expressed in our study such as : [IIIa'], [Iia'],[IIb'] and [IIIc]. More importantly, if the model is forced to select only compounds with [br]i>10% or even 5%, correlations to MAP and MAAT disappear (best R^2 around 0.17 and 0.14, respectively).

- Last, the main purpose of this manuscript is to develop a common methodology for both pollen and GDGT modeling using statistical selections of modern analogues and without any eco-physiological consideration. This choice was made based on the lack of constrains on biological processes driving GDGT production. This holds true for pollen, a proxy where the relation between climate – vegetation and pollen production is definitely much restrained. The biologically blind method is thus useful to avoid over-explanations of causes and consequences.

Applied Change: To clarify these issues, the 2nd point of the steps at the end of the introduction (L. 94) has been modified in :"Evaluation of the match between actual bioclimate environments and associated pollen rain and biomarker assemblages based on mathematical criterion without any eco-physiological considerations."

- Even if all models presented in this study, MR-GDGT models included, are made on eco-physiological blind test, some physical laws governing these models can be derived.
- First, the main molecules involved in the mr-models are overall matching with the RDA vectors. For instance, the $MAAT_{mr}$ models apply + $[IIIa']$ and – $[IIIa]$, consistently with the GDGT-climat RDA. This indicates that, on our data-set at least, the mr-models follow the climatic forcing displayed in the RDA analysis. Table Fig.2 (in the interactive comments) presents the 4th mr-GDGT model selected as the better representation of Sibero-mongolian climate. br-GDGT compounds are ordinated by decreasing proportions. Number and sign in cells show the importance of each br-GDGT in the model and if they are positively or negatively used in the model.
- On the table S1, except for [IIb'], all the compounds change their sign when used with another climatic parameter. For instance [IIIa] is positively correlated with

MAAT and negatively with MAP. It is consistent with the anti-correlation between MAP and MAAT (Annex Fig. B1).

- Then, we observe that the main variables for MAAT are gathered in the group G1 mainly composed of penta and hexamethylated brGDGTs, while the MAP in G2 is mainly based on tetra and pentamethylated brGDGTs (table Fig. 2 in the interactive comments). This group G2 is also composed exclusively by compounds with 2 (b) or 3 (c) cycles. The MAP reconstruction is then leaded by the cycled molecules. These componds are known to be linked to pH (Damste et al., 2016, Weijers et al., 2007b) with an increasing number of cycles for basic soils (pH>7). The basic soils are often associated with low precipitation area because of the weak weathering effect (Dregne et al., 1976; Haynes et al., 1989).

Applied Change: Paragraph 4.2.3 (L. 324) : "*Both* $MAAT_{mr}$ *models infer on a positive contribution of [III'a] and a negative contribution of [IIIa], which confirm these models are eco-physiologically consistent with RDA results. Moreover, except for [IIb'], all compounds are positively correlated with MAAT and negatively with MAP, in accordance with MAP - MAAT anti-correlation.*" Paragraph 5.4 (L. 410) "*(...) arid soils favor 6-Methyl by pH raising due to the low weathering effect of the weak precipitation (Dregne et al., 1976; Haynes et al., 1989)*"

-Lastly, what is missing from this manuscript is an application of these novel calibrations. Do they provide sensible climatic signals when applied to a downcore record? If the authors do not have a downcore record, is there a published record that this calibration can be applied to?

Response: We acknowledge the comment by the referee, the application of these calibrations to a paleorecord is the ultimate goal of this study. We first considered

submitting the two sets of data in the same manuscript but the resulting text was too long to properly address the issues raised by the calibration. We chose to first describe in details the methodology as well as the advantages and pitfalls of statistical treatments for deriving MAAT and MAP calibrations in arid areas. This will allow to document in a second step, the implications of this calibration exercise in terms of paleoclimate reconstructions.

Specific comments:

Line 6: delete "extremely cold dry"

Response and applied changes: Modified accordingly

Line 7: is the livestock grazing statement relevant? It does not appear to come back in the discussion, delete?

Response and applied changes: Modified accordingly. The grazing is actually particularly relevant for the understanding of alpine and semi-desert vegetation and consequently the pollen rain. However, since we did not focus on Non Pollen Palynomorph (NPP), we did not develop much this point in the present manuscript.

Line 16: add "environmental variations in Mongolia and Siberia"

Response and applied changes: Modified accordingly.

Line 52 and 55: brGDGTs

Response and applied changes: Modified accordingly.

Line 55: also cite other recent brGDGT calibrations papers, for example (Wang et al., 2019)

Response and applied changes: Modified accordingly: Wang et al., 2019 and 2020 on attitudinal transects.

Line 62-63: I don't think we show this in our 2018 paper. Delete sentence or change reference.

Response and applied changes: We were referencing to "*Whether this is related to changes in the source organism's brGDGT distribution or due to changes in the bacterial community composition is currently unclear.*" which is not the main subject of the article but raised similar doubts. The sentence has been modified into "*Moreover some studies have focused on the variations in the bacterial community structure (Xie et al., 2015), the bacterial group responses to environmental changes (Knappy et al., 2011) and the GDGT occurrences in different bacterial communities (Liu et al., 2012b) to determine the possible community structure impact of GDGT abundance.*" (L. 65)

Introduction needs some rewriting to create a more natural flow between the different paragraphs. At the moment the introduction jumps from pollen to brGDGTs and back without a clear connection between the different paragraphs. A good example is the sentence in Line 71 that sort of floats by itself with no connection to the previous

sentences or the next paragraph. The end of the introduction with a clear outline of the approach is good.

Response and applied changes: We agree with this general comment on the introduction. The link between the paragraphs have been smoothed.

Also, I think somewhere in the introduction the authors need to introduce the 5,6,7 methyl brGDGTs and what they mean (For example citing De Jonge et al., 2013; Ding et al., 2016). Because at the moment their use (e.g. line 276) comes a bit out of nowhere (need also somewhere in the methods explain the use of ' and '' for 6, and 7-methyl brGDGTs).

Response and applied changes: The 5th paragraph of the introduction dedicated to GDGTs have been enriched by :"In particular, the methylation degrees, ratios of 5, 6-methyl (De Jonge et al., 2013) and 7-methyl isomers (Ding et al., 2016) reacts to environment forcing : the 5-methyl correlates mainly with temperature (Naafs et al., 2017), while 6 and 7-methyl seem to react to moisture and pH changes (Yang et al., 2015, Ding et al., 2016)."(L. 69)

Line 265-270: this section needs a bit of re-writing (and maybe thinking). We know isoGDGTs are also produced in soils and peats, not just in lakes and not only in the water column. So that is not the reason that you see no clear correlation with climate parameters. See the discussion in (the supplementary information of) (Naafs et al., 2018) on the distribution of isoGDGTs in peat and the lack of correlation with temperature/pH. It is interesting that in these samples from dry environments crenarchaeol is abundant because the abundance of crenarchaeol in soils/peat has been inferred to indicate dry conditions (see for example Zheng et al., 2015), I suggest the authors expand on this.

Response: We agree with this observation. We have tried the check the crenarcheol-MAP relationships, and we did not find any. The best (but weak) result (Figure 3 in the interactive comments)) found linked the ratio crenarcheol/regioisomer.

Applied changes : (L. 82)"*Iso-GDGT pattern in lake sediments do not really diverge from surface samples which leads to postulate that the in-situ production of iso-GDGTs in shallow lakes like MMNT5C12 is reduced (Fig. 4.A). Then, it appears that the iso-GDGT soil-produced are dominated by crenarcheol in accordance with studies on aridity impact (Zheng et al., 2015). However, no relationship exists between [crenarcheol] and MAP (R^2 = 0.14, p − value > 0.005). The putative regio-isomer reaction linked to MAP (Buckles et al., 2016) is not evidenced in NMSDB.*"

Line 274: I don't understand this sentence

Response and applied changes: The text has been modified (L. 292): "*Particularly, the PC1 represents 22.77 % of the total variance and distinguishes two opposed poles: the 5-methyl group (mostly with PC1 >-0.3 associated with steppe-forest and forest sites) and the 6, 7-methyl groups on the far negative PC1 values associated with steppe and desert sites.*"

Figure 4: change legend to state "lake sediments, n=65"

Response and applied changes: Modified accordingly

Line 279: what kind of surface samples? Soil surface?

Response and applied changes: To emphasize the influence of sample type, the paragraph has been fully rewritten: "The sediment samples from the lake MMNT5C12, used as past sequence comparison, are more homogeneous than the soil surface samples, especially when compared with the moss polsters (wide variability (Fig. 4B)). Generally, soil samples are more relevant analogues to lake sediments than moss polsters (especially [IIIa'], [IIa] and [Ia] relative abundances in Fig.4B). This variability shows an influence of the sample type on br–GDGT responses. On the other hand, sample type also bears climate and environment information, since soils and moss polsters originate mainly from steppe to desert environments and forest/alpine meadows, respectively."

Line 297-298: On what basis were these 9 selected?

Response and applied changes: The 15 models correspond to the best fitting model for each parameter added. Then we pick-up 9 models in the 15 whenever the addition of a parameter did not change significantly the statistical values (R^2, AIC and RMSE) more than a decimal of the previous model (with one parameter less). The sentence paragraph 4.2.3 have been modified to "*Within the 15 models (one model for each parameter addition), the 9 more contrasted ones were selected for discussion (Table 2).*"(L. 318)

Expand Section 5.3: I think the assumption for this section is flawed. Of course, a local calibration based on a certain set of surface samples will have a better correlation with the MAAT then a global calibration applied to these surface samples. You chose your local calibration using these same samples.

Response and applied changes: This observation is true for the cross-values made on samples also used for the calibration (the right part of all the panels A1, B1 and C1 on the fig.7) but it is not the case anymore for the "Cross-value" section of this same figure. Indeed, the 6 samples selected from the MMNT5C12 cores are all independent from our local br-GDGT calibration. The discussion of section 5.3 is based upon the panels of this graph. Since the discussion is based on an independent set of cross-value samples, the assumption should not be affected. We have tried to clarify by adding the following sentence: (L. 368) "*We tested both approaches on our datasets with a cross-value effectuated on the NMSDB-independent set of MMNT5C12 core samples*" at the beginning of part 5.3.

Line 379: also see discussion in (De Jonge et al., 2014; Naafs et al., 2017) on brGDGTs in dry soils

Response and applied changes: Some of the observations made on our data set corroborate the discussions in De Jonge et al., (2014) and Naafs et al., (2017), we have mentioned it in different parts of the manuscript:

- In the results (part 4.2.2, L. 304) "*The lower MAP match with 6 or 7-Me GDGTs, such as [IIIa'], [IIa'], [IIa"] in line with De Jonge et al., (2014b).*"
- In the discussion (part 5.4, L. 407) : "*First, the commonly used br–GDGT indexes (MBT and CBT) are not relevant for arid areas with $MAP < 500mm.yr-1$ (Dirghangi et al., 2013; Menges et al., 2014) because of the relationships between low soil water content and soil br–GDGT preservation and conservation interfering with that of br–GDGT / climate parameters (Dang et al., 2016). The MAAT models built on MBT and MBT' indexes provide colder reconstructions (Fig. 7.C2) as it has been shown De Jonge et al. (2014b) because the arid soils favor 6-Methyl (by pH raising) and drive to the MBT flattening. This explain*

the colder than real climate reconstructions provided by the $MAAT_{Ding}$ *and* $MAAT_{MBT'-DJ}$ *calibrations.*"