Response to Interactive comment on **"OPTiMAL: A new machine learning approach for GDGT-based palaeothermometry"** ***by*** **Yvette L. Eley et al.**

Formatting notes:

Reviewers / Other comments are in bold italic

Our responses are in plain type

Proposed changes in manuscript or quotes from existing text are in italic

Response to Open Comments of HUAN YANG

This manuscript presents a new approach, 'OPTiMAL' to improve the accuracy of palaeo sea surface temperature reconstruction, in particularly focusing on the GDGT data from greenhouse worlds. The effort of improving the sea surface temperature reconstruction is welcome. As an organic geochemist without enough knowledge of machine learning, it is difficult for me to understand some parts of the manuscript as most parts of the discussion show how the model was established and what the performance of this model was. I can understand the rationale of the model used in this manuscript: GDGT data should have 6-dimensional information and machine learning approach used in this study can capture the 6-dimensional information, which appears to be better than one dimensional information shown by TEX86. However, I strongly suggest the authors should be cautious when discussing the TEX86 and its derivatives because these proxies are still applicable in most cases and in most work of palaeoSST reconstruction in the greenhouse world, these proxies are still applicable.

We thank Huan Yang for their comments regarding the need to improve SST reconstructions. We have gone through the manuscript again, to ensure clarity of phraseology. We note the suggestion that we should exercise caution when discussing TEX_{86} and other similar indices, and the argument that even in greenhouse worlds, these proxies are still applicable. In this context we refer back to our response to Tierney above:

"We do not wish to stop people using GDGT-based thermometry for the reconstruction of greenhouse climate states. We simply wish to urge caution in the application of this method when the fossil GDGT assemblages, from any time period, are strongly non-analogous to the modern calibration data on which this proxy rests. As we demonstrate this appears to be an increasing problem with increasing sample age, but it does not preclude the use of this proxy in greenhouse climate states where the fossil data are well-constrained by the modern calibration. Again, this was a primary goal of this paper, to separate well- from poorly-constrained SST estimates; it is a concern to us if the community do not wish to make the same distinction but that is yet to be decided."

The authors should also carefully check the manuscript as there are a number of typos. In particular, the reference list should be checked carefully. Some minor points are appended below.

Line 52 'LC-MS' Full name should be shown here.

We will amend this in the final revised submission

Line 60-61 References should be arranged in the time order.

We will amend this in the final revised submission

Line 63 Zhaung should be Zhang.

We will amend this in the final revised submission

Line 73 'in response to these criticisms' Better to use other words.

We are not sure why the reviewer feels that these words are inappropriate, and therefore we have not amended them

Line 77 'Kim et al. 2010' should be 'Kim et al., 2010'.

We will amend this in the final revised submission

Line 90 'Hollis et al. 2012; Dunkley Jones et al. 2013; Lunt 2012' should be 'Hollis et al., 2012; Dunkley Jones et al., 2013; Lunt 2012' . The references should be listed in the time order.

We will amend this in the final revised submission

Line 95 Add comma after 'et al.' Line 96 Delete the comma after 'production'.

We will amend this in the final revised submission

Line 97 'ð˙IS´ Gð˘ ˙IRÿð ˘ ˙IS´ N86L is no longer regarded ´ as an appropriate tool for palaeotemperature reconstructions'. This proxy is still applicable in most marine regimes and could be used to infer SSTs.

This comment relates to TEX_{86}^{L}. A recent seminal study on proxy methodologies for paleoclimate reconstruction in deep time (Hollis et al., 2019) highlights that TEX_{86}^{L} does not accurately reflect the degree of cyclization of GDGTs, and therfore lacks a biological rationale. Equally, TEX_{86}^{L}shows enhanced sensitivity to biases driven by contributions from other subsurface archaea (Hollis et al., 2019). We therefore do not agree with this comment that TEX_{86}^{L} is "applicable in most marine regimes" and will not amend the sentence in our revised manuscript.

Line 103 'BIT' should be shown in full name

We will amend this in the final revised submission

Line 104 Add comma after 'et al.'.

We will amend this in the final revised submission

Line 131 'crenarchaeol regioisomer'

We will amend this in the final revised submission

Line 192-193 I think data from Tierney and Tingley (2015) do not cover all the published core-top GDGT data. A number of other data published recently should also be included.

In the first instance we stick to the Tierney and Tingley (2015) data to be comparable to the BAYSPAR calibration dataset, but we will explore further integrations of new core top data.

Line 228 Delete 'the crenarchaeol regio-isomer' and you can use cren' here.

We will amend this in the final revised submission

Additional references (not found in our original submission) referred to in our response – these will be incorporated into our final revised submission:

Bale, N. et al. (2019) Applied and Environmental Microbiology 85(20) e01332-19
Cadillo-Qiuroz, H. et al. (2012) PLOS Biology, https://doi.org/10.1371/journal.pbio.1001265
Dunkley Jones, T. et al. (2013) Earth-Science Reviews, 125, 123-145
Elling, F. et al. (2017) Environmental Microbiology 19(7), 2681–2700
Hollis, C. et at. (2019) Geosci. Model Dev., 12, 3149–3206
Liu, X-L. et al. (2014) Marine Chemistry, 116, 1-8.
Lunt, D. J. et al. (2012) Clim. Past Discuss., 8, 1229- 787 1273.
Qin., W. et al. (2015) PNAS 112 (35) 10979-10984
Schouten, S. et al. (2007) Organic Geochemistry 38, 1537-1546
Wuchter, C. et al. (2004) Paleoceanography 19, PA4028, doi:10.1029/2004PA001041, 2004
Zhang, Y. G. et al. (2016) Paleoceanography, 31, 220-232
Zhu, J. et al. (2019) Science Advances 5 (9), eaax1874