

Review: BG-2019-345

In the manuscript “Comparison of the $U_{37}^{K'}$, LDI, TEX_{86}^H and RI-OH temperature proxies in the northern shelf of the South China Sea,” Wei et al. evaluate spatial gradients in four organic paleotemperature proxies across this coastal region. The authors specifically sought to determine the biological sources of the four classes of lipid biomarkers related to the title proxies (alkenones, long-chain diols, isoprenoid GDGTs, and OH-GDGTs, respectively) and any possible seasonal biases in temperatures reconstructed from sedimentary distributions of the lipids. The manuscript offers insights to the distributions of paleoclimate-relevant lipids in the modern, expanding upon the results of similar studies in the region. The results of this study are particularly relevant for the development of the newer organic paleotemperature proxies based on long-chain diols and hydroxylated GDGTs. Though this work has the potential to inform interpretations of downcore paleotemperature reconstructions from SCS sediments, I find the authors fail to clearly draw this connection themselves. Overall, I feel that the manuscript needs to be significantly revised before it should be considered for publication in Biogeosciences. Specifically, the manuscript could be strengthened with additional statistical analyses that draw more robust connections between environmental variables and lipid distributions as well as with a more in-depth discussion (or at least acknowledgement) of the many factors known to influence lipid production in marine organisms (e.g. growth rates, oxygen concentrations, lateral transport, export efficiency, water column structure) in addition to the few already mentioned in the manuscript.

General Comments

The English in this manuscript needs to be improved to increase the readability of the text. The authors are advised to carefully review the entire manuscript for grammatical and syntax errors. Some examples of language that needs improvement are:

Grammatical Errors:

Line 35: Need to change “were synthesized” to “are synthesized.”

Line 241: Authors refer to sediment trap studies (plural) but only include one reference.

Awkward Syntax:

Line 13-15: “The applicability of these proxies has been examined in the South China Sea, but most of these studies were focused on a single proxy and hence did not allow for a direct comparison between them.”

Lines 49-50: “Due to the distinctive ecology of their source organisms, these temperature proxies differ in reflecting water temperatures in terms of, e.g., water depth and seasonality.”

Lines 321-323: “It should be noted that it remains unclear what causes the different iGDGTs distribution between those two eco-types, and the depth boundary to separate the two, likely 200–300 m, is not exactly determined (Jia et al., 2017; Kim et al., 2015, 2016).”

The discussion section on the seasonal bias of $U_{37}^{K'}$ is weak. Reported measured SSTs approach the upper limits of the Conte et al. (2006) calibration so a nonlinear relationship between $U_{37}^{K'}$ and

SST is likely. Linear calibrations, including the one from Conte et al. (2006) used in this study, are hindered by a tendency to underestimate SSTs in warm regions. As such, it's possible that the apparent bias towards production of alkenones during cool-seasons inferred from $U_{37}^{K'}$ -reconstructed temperatures might be an artifact of this limitation. An example of this in the SCS is illustrated in Tierney and Tingley (2018). Furthermore, support for the authors' hypotheses on the role of nutrients in driving the ecology of alkenone-producers in the SCS is lacking. Why not use nutrient and salinity data provided by the WOA to support your hypotheses on the effect of the PRE on the study region? According to the paper from Chen et al. (2007) cited in this study, alkenone-producer populations in the SCS are more mesotrophic-to-oligotrophic and only outcompete diatoms when nitrate concentrations are relatively depleted. Chen et al. (2007) further state that haptophyte algae populations are sensitive to water column structure, a point that you don't consider in your discussion.

The authors' discussion on iGDGTs is also an incomplete representation of current knowledge on the TEX_{86} proxy. First, the authors mention that the correlation between TEX_{86}^H -reconstructed SSTs and observed SSTs could be improved with a "shallow-water" calibration, yet then proceed to apply the Jia et al. (2017) calibration which is exclusively based on sediments from > 329 m water depth. Furthermore, the Jia et al. calibration was calculated against water column temperatures across the upper 30-125 m whereas a number of samples in this study were collected at depths < 30 m. The authors should consider re-evaluating their data using BAYSPAR (Tierney and Tingley, 2015) *cf.* de Bar et al., 2019 (doi:10.1029/2018PA003453). Second, it is well-known that Thaumarchaeota inhabit a range of depths in the marine water column, but most typically reside at the base of the euphotic zone. A previous study in the SCS identified the depth of maximum Thaumarchaeotal abundance ca. 50 m (Dong et al., 2019), and line 50 of this manuscript states that iGDGTs in the SCS are likely produced between 30 m - 125 m. As many samples in this study lie above these depths, it would be interesting to know how iGDGT concentrations vary across the region and how accumulation rates of sedimentary iGDGTs relate to measured TEX_{86} . The authors also reference Zhang et al. (2017), which found that iGDGT distributions in the East China Sea from locations at < 70 m water depth were significantly impacted by non-temperature influences such as nutrient from upwelling, lateral transport, or resuspension of sedimentary material. These results have significant implications for the interpretation of the data presented here, yet these factors are not thoroughly acknowledged.

The OH-GDGT discussion is complicated by the lack of acknowledgment that the extraction technique employed in this study may have biased the results. Yang et al. (2018) demonstrated that ultrasonic extraction of GDGTs from South China Sediments resulted in significantly lower apparent concentrations of OH-GDGTs relative to samples extracted following a Bligh-Dyer method. In Yang et al., decreased extraction efficiency of OH-GDGTs using an ultrasonic method additionally led to significant biases in SST reconstructions using the RI-OH proxy. You should acknowledge this in the manuscript in the methods or discussion sections on OH-GDGTs.

For all of the proxy data presented in this manuscript, it would be beneficial to see it placed in the context of other regional studies, similar to Figure 8.

Lastly, the figures do not represent the data well and need to be updated, as do the figure captions which I also found generally uninformative. Figures 2, 3, and 4 are especially difficult to interpret. In Figure 2, the use of the same colors for both the WOA-derived SSTs and the markers related to the proxy data is confusing. This figure could be improved by splitting up the data, for example by

having a 4-panel figure with 1-panel per proxy. Figure 3 would be more useful as just a single map showing the spatial trends in the %C₃₂1,15 index that is referenced in Line 198 instead of plotting the fractional abundance of each of these 4 diols. For Figure 4, consider averaging the fractional abundances for certain depth classes then plotting the mean for that group in a bar graph similar to your Figure 5. Again, since both the spatial and depth patterns are important in this study, I think it would be best to plot each index in panels 4b and 4d individually as a map similar to your Figure 3.

Specific comments:

Line 39: Cite Kim et al. (2010) after referring to TEX_{86}^H and TEX_{86}^L .

Line 40-41: Crenarchaeol has 4 cyclopentane moieties as well as the cyclohexane ring, so you should rephrase this sentence to something like “...(iGDGTs) containing 0-3 cyclopentane moieties (GDGT-0, 1, 2, 3, respectively) or 4 cyclopentane moieties with an additional cyclohexane moiety (crenarchaeol and its isomer, Cren and Cren’, respectively)...”

Line 41: Recent studies (Sinninghe Damsté et al., 2018 doi:10.1016/j.orggeochem.2018.06.005; Liu et al., 2018 doi: 10.1016/j.orggeochem.2017.09.009) have determined that the crenarchaeol isomer is not actually a regio-isomer, so you should update your text by removing all instances of ‘regio.’

Line 44: Though there is still a lot to learn about the biological source of LCDs, I don’t agree with the statement that the source is “albeit not unambiguously identified yet” as there are several papers that have isolated LCDs in culture studies of diatoms and eustigmatophyte algae, in addition to many phylogenetic studies that link the lipids to source organisms in natural environments.

Line 45-48 Include references to Elling et al., 2014, 2015 & 2017. Nevertheless, I don’t think you represent current knowledge on the source of OH-GDGTs fairly here. See Lipp et al., 2009; Zhu et al., 2016; Sollai et al., 2019.

Line 167-170: As nearly half of your samples were collected in years not represented in the WOA13 V2 product, I recommend you update the manuscript with the WOA18 data that was released this summer. Furthermore, given that the studies you contrast your results to later on calculate seasonal averages from different months than those defined in the WOA product, you should use the monthly data from the WOA18 instead of the pre-defined seasonal means to strengthen the comparisons you draw in the discussion section.

Line 177: You use the acronym “WD” yet this acronym was never defined previously in the text.

Line 205/Section 3.4: You should separate the results related to iGDGTs and those related to OH-GDGTs.

Line 223-224: Are these relationships significant?

Line 233-234: Why do you refer to the Chinese Marginal Sea here instead of the South China Sea?

Line 235-236: It is confusing that you refer to residuals here when the figure you reference (Fig

2) does not show the Proxy – Obs. SST residuals.

Line 239: Include references to culture studies that support this statement.

Line 244-245: You really should discuss why you think your results indicate that $U_{37}^{K'}$ -SST are biased towards spring temperatures as there is nothing in Figure 2 that demonstrates this. You could do a simple linear regression between $U_{37}^{K'}$ -derived temperatures and seasonal SSTs and if there is a significant relationship with observation spring SSTs, then your claims are valid.

Line 270: Either here or in the methods section you should provide more details on how you conducted this statistical analyses.

Line 279: Based on your above discussion on the different sources of these three lipids and the results of the previous studies on LCD distributions in coastal environments that you cite, this supposition about an opposite relationship between $C_{28:1,13}$, $C_{30:1,13}$, and $C_{32:1,15}$ diols and temperature is unlikely and seems unnecessary to include.

Line 285 - 287: The statement explaining why a threshold of $\%C_{32:1,15} < 20\%$ was used from Lines 288-290 should be moved here.

Line 305: Replace “methane-related” with something more accurate such as “...iGDGTs from archaea involved in methane cycling...”

Line 306: Please indicate what “substantially elevated” values for the $[2]/[Cren]$ and $[0]/Cren$ indices are as you do for the MI.

Lines 309-312: Another paper you cite elsewhere in the text, Zhou et al. (2014), concluded that brGDGTs in the PRE are also likely derived from in situ production in the river rather than solely originating from erosion of catchment soils.

Line 321-322: The difference in iGDGT distributions between ‘deep’ and ‘shallow’ Thaumarchaeota eco-types is due to the use of different enzymes for iGDGT synthesis (cf. Kim et al., 2016 doi: 10.1016/j.gca.2015.09.010; Villanueva et al., 2014 doi: 10.1111/1462-2920.12508).

Line 339-343: In Kim et al.’s 2008 paper, the authors note that the difference in their TEX₈₆ calibration for core top sediments from depths < 200 m relative to the calibration for the entire data set is negligible, likely because contribution of iGDGTs from deep-dwelling archaea to the sediment floor is minimal relative to the contributions from shallow-dwelling Thaumarchaeota, a point that has been highlighted in many other studies. As such, I don’t believe this is the cause of the mismatch between the TEX₈₆^H-reconstructed temperatures and observations you report in your manuscript.

Line 390: In Line 315 you draw the opposite conclusion – that your samples are not appreciably impacted by TEX₈₆^H?