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Calibration of bacterial 3-hydroxy fatty acid based palaeoclimate proxies in global soils

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3-Hydroxy fatty acids (3-OH-FAs), derived from Gram-negative bacterial outer membranes, have received recent attention for their potential as both: a) terrestrial palaeoclimate proxies (Wang et al., 2016; Huguet et al., 2019;); and b) marine sea-surface temperature proxies (Yang et al., 2020). This potential was highlighted by the application of 3-OH-FAs to a Chinese stalagmite to reconstruct temperature and hydrological changes over the last 9000 years (Wang et al., 2018). Initial studies from altitudinal transects of contemporary soils - correlating bacterial 3-OH-FA compositions to air temperature and pH – have showed promising results, but also highlight regional differences in calibrations (Véquaud et al., 2020). Thus calibration based on globally distributed soil sample set is thus needed to test the wide-spread applicability and improve the estimation accuracy of 3-OH-FA based proxies.

We find that the ratio of *anteiso* to *normal* 3-OH-FAs of the C_{15} or C_{17} homologues (RAN_{15} or RAN_{17}) shows a significant linear relationship with mean annual air temperature (MAAT) ($R^2 = 0.48$ and $R^2 = 0.41$) in 186 global soils. Additionally, the negative logarithm of the ratio of the summed *iso* and *anteiso* to the total amount of *normal* 3-OH-FAs (RIAN) is primarily related to the soil pH ($R^2 = 0.66$). Machine learning tools confirm the general relationships observed in the empirical equations and derives several alternative Gaussian Process (GP) emulator models for reconstructing MAAT and pH which give higher R^2 values (0.66 for MAAT; 0.63 for pH) and lower RSME values (3.5°C for MAAT; 0.76 for pH) compared to simple linear regressions. However, significant regional differences suggest that local or regional calibrations may be preferable to a singular global calibration. We recommend that workers explore and apply both global and regional scale calibrations (empirical and machine learning based) to paleoclimate data-sets during this nascent stage of 3-OH-FA development for palaeoclimate.

References

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