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Enzyme adaptation and habitat thermal legacy: from microbiome adaptation to climate change to smart selection of enzymes with thermal characteristics

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PURPOSE OF THE ABSTRACT

Global warming is one of the biggest concerns of modern society as it is one of the main hazards for healthcare. But, climate change is also altering the ecological patterns and the way temperature would select the skills of cellular building blocks, such as enzymes. We hypothesize that environmental mean annual temperature (MAT) contributes to drive the adaptability of marine microbial communities by tuning the thermal plasticity of their enzymes, and that such plasticity is fine-tuned further by environmental temperature variability [1]. To test this hypothesis, we studied the enzymatic thermal response of marine microbial communities at a global geographical scale across different locations within a broad latitudinal gradient and different MAT conditions (-1.4 to 28.5 °C). Here, the following meta-data are presented for active proteomes and 233 individual enzymes: 1) the optimal

temperature (T_{opt}) for activity of seven functionally-independent enzyme classes; 2) the thermo-stability, by meaning of the denaturation temperature (T_d) patterns; and 3) the phase transition temperature (T_p), a computational measure of structural flexibility. The generated meta-data were analyzed as a function of the environmental parameters at the site from which the enzymes originated, namely, the variability in MAT, salinity, pH, hydrostatic pressure or light received. To also consider the thermal variability (TV), the response of enzyme activity (T_p and T_d) to TV was evaluated and compared with the microbial growth characteristics in three adjacent marine sites with same MAT but with different TV throughout all the seasons.

Our results showed that microorganisms better adapt to different thermal conditions by selecting thermally-adapted enzymes (through genetic adaptation, e.g., new genes) rather than selecting enzymes with broad thermal tolerances. At the same time, microbial communities living in environments with a wide temperature variability have higher thermal plasticity, in consonance with the thermal legacy of their enzymes. The fine-tuned response of microbial communities to temperature change is thus controlled, at least in part, by the selection of enzyme variants that are capable of being active under more variable temperatures.

From a climate change adaptation point of view, this implies that while the adaptation of microbial communities to temperature change appears to be mediated by the selection of thermally adapted enzymes, the extent of this adaptation also depends on temperature variability. This should be considered when modelling the response of marine and coastal microbiota to climate change, as projections suggest that more than 85% of ecosystems and 16% of their microbes will be influenced either directly or indirectly by climate change [2]. From a more technical point of view, the fact that a significant correlation ($p < 0.05$) between the computed T_{opt} , T_d , T_p , and the MAT and TV from the site where each enzyme was retrieved, implies that these parameters, particularly the T_p , which can be calculated from sequence information through constraint network analysis, and the environmental MAT/TV information, can be used as motifs/parameters for implementing sequence-based smart search of enzymes fitting thermal needs with which to implement the industrial reconversion needed to complete the green transition and to achieve climate neutrality.

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FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

enzyme discovery | computational methods | thermal legacy | marine microbiome

BIBLIOGRAPHY

1. Marasco, R., Fusi, M., Coscolín, C. et al. Enzyme adaptation to habitat thermal legacy shapes the thermal plasticity of marine microbiomes. *Nat Commun* 14, 1045 (2023).
2. Guerra, C.A., Delgado-Baquerizo, M., Duarte, E. et al. Global projections of the soil microbiome in the Anthropocene. *Glob Ecol Biogeogr* 30, 987-99 (2021).