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Environmental conditions control on molecular configurations of isoprenoid glycerol dibiphytanyl glycerol tetraethers: insight from molecular dynamics simulation

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Isoprenoid glycerol dibiphytanyl glycerol tetraethers (isoGDGTs), served as important biomarkers in the field of marine biogeochemistry, is used to understand the Earth's history according to their diverse molecular structural information. However, the ambiguous mechanism on structural changes of isoGDGTs has limited the accurate application of their inverting environmental information. Here, we use molecular dynamics (MD) simulations to investigate configuration and structural total energy of individual isoGDGT under the control of temperature, in order to provide a theoretical explanation for the configurational changes of individual lipid under the influence of environmental conditions. We also compare the MD simulated results with relative abundances of individual isoGDGT from environmental surveys to validate the reliability of our modeling results. The same pattern between the change of structural total energy of GDGT-0 and GDGT-cren provided by MD simulations and their relative abundances collected from global data with the growth temperature, indicating the mechanism of temperature influencing configurations of isoGDGTs attributes to differences in the energy demands of synthesizing individual lipid by Archaea from a physiological perspective. The molecular specific surface area (MSSA) of equilibrium configurations of GDGT-1~3 and GDGT-cren' is proposed to theoretically explain divergent TEX_{86} signatures in high and low latitude regions that have been controversial points so far, which may be as a result of temperature exerting selective degradation on different configurations of isoGDGTs under burial and deposition environments further influencing the TEX_{86} values. An MSSA index is established to assess the suitability of TEX_{86} before the application of reconstructing SSTs. Our work provides a molecular configurational and theoretical explanation of how temperature influences structural changes in isoGDGTs from both a physiological and a preserved perspective.