THE TEX_{86} INDEX IS A NEW TOOL TO RECONSTRUCT ANCIENT SEA SURFACE TEMPERATURES

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When we want to understand better what to expect in the future, we have to learn from the past. This is also true for the present change in our climate. To do this, we use organic compounds preserved in sediments from ancient microbial communities. The structures of the compounds give information about the environment in which the organisms possessing these compounds lived. One of the most crucial factors is the reconstruction of past sea surface temperatures (SST). Some groups of compounds that are part of the cell membranes of organisms adapt their molecular structure in order to maintain similar membrane properties over a range of water temperatures. When these changes can be calibrated experimentally with cultivated living organisms, it becomes possible to reconstruct records of palaeo-temperatures from dated sediment cores. Here we present our newly developed TEX_{86} index (TEX_{86}=Tetra Ether IndeX of lipids with 86 carbon atoms), which is based on the tetra-ether lipids from the cell membranes of a particular branch of Archaea: the marine Crenarchaeota.

Marine Crenarchaeota are Prokaryotes that belong to the domain of Archaea. Recent molecular biological work showed that the group of the marine Crenarchaeota is ubiquitously distributed and comprises ca. 20% of the picoplankton in the world's oceans. The membrane lipids of marine Crenarchaeota consist of a unique group of compounds: the glycerol dibiphytanyl glycerol tetraethers (GDGTs, Fig 1). Culture experiments have shown that the hyperthermophilic Crenarchaeota, which live at temperatures of 60-100°C, change their relative distribution of the (5 carbon) cyclopentane rings in their membrane lipids as a function to temperature. With this mechanism, they keep the properties of their cell-membrane constant over a range of temperatures. For the adaptation of the marine Crenarchaeota to temperate seas such as the North Sea and the Wadden Sea, another structural adaptation to the GDGT molecules has occurred in the form of an extra cyclohexane ring (with six carbon atoms) This compound was named crenarchaeol and its structure is drawn as no. V in fig 1.

Archaeal lipids in sediments

The distribution of GDGTs from marine Crenarchaeota in core top sediments derived from different geographic locations correlates well with SST. In cold areas the GDGT distribution is dominated by GDGT (I) (Fig. 1) and crenarchaeol (V). In warmer regions the GDGT distributions differ substantially, as crenarchaeol becomes the most

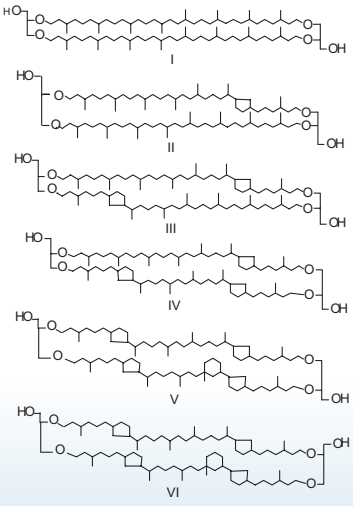

Fig. 1. Molecular structures of membrane lipids of marine Crenarchaeota. The compounds I-VI are GDGTs with 0-4 cyclopentane rings. Compound V is crenarchaeol and VI is a regio-isomer of crenarchaeol.

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Fig. 2. Set-up of the experiment (carried out in darkness).

abundant GDGT. Moreover, the GDGTs with 1-3 cyclopentane rings (II-IV) increase, and a regioisomer of crenarchaeol (VI) is also detected. The relative GDGT distribution can be expressed as an index of the concentrations of the GDGTs II, III, IV and VI. We named this the TEX_{86} index, which is defined as follows:

$$TEX_{86} = \frac{III+IV+VI}{II+III+IV+VI}$$

Thus, only GDGT II occurs exclusively in the denominator of the index! The correlation of the TEX_{86} index to the annual mean SST resulted in the following linear equation for a number of core-top sediments from different areas:

$TEX_{86} = 0.015*T+0.28$, (r^2=0.92) with T = annual mean SST (in ºC).

However, an observed high correlation of the GDGT distribution in sediments with SST can never provide direct causal evidence that marine Crenarchaeota adapt their physiology exclusively to the temperature of the ambient seawater. For instance, variations in salinity may also play a role.

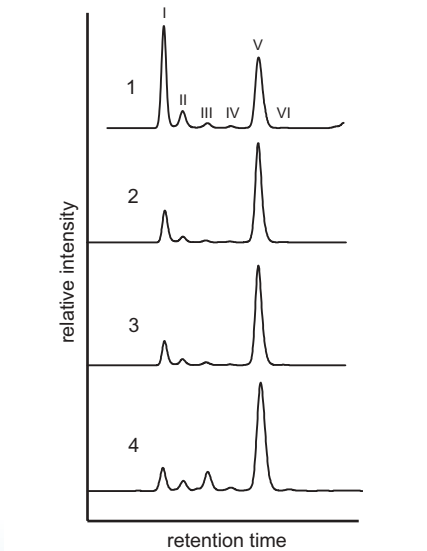

Fig. 3. HPLC-base peak chromatogram of membrane lipids of marine Crenarchaeota as recovered from the mesocosm experiments. The roman numbers correspond to the structures in Fig. 1. Mesocosm tanks were incubated at different temperature and salinities (1) 10°C and 27‰, (2) 25°C and 27‰ (3) 25°C and 35‰ and (4) 35°C and 27‰.

Calibration of the TEX_{86} in laboratory cultures

Crenarchaeota cannot yet be grown in pure cultures. Therefore North Sea water was incubated in 20L mesocosm tanks (Fig. 2.) over a range of temperatures (5-35ºC) and salinities (27-35‰) (Fig. 3). The experiments were carried out in the dark to prevent the growth of algae. As expected, an increase in the number of cyclopentane moieties in the crenarchaeotal membrane lipids with increasing water temperature could be observed (Fig.3). In contrast, the differences in salinity did not show any effect on the membrane lipid distribution (Fig.3) and thus salinity does not disturb the temperature signal. The TEX_{86} values from our incubations

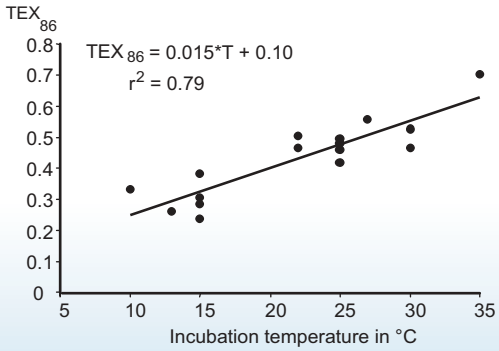

Fig. 4. Correlation of the TEX_{86} index with seawater temperature in the mesocosm experiments.

showed a significant linear correlation to incubation temperature (Fig.4) with the same slope of 0.015 as obtained from the sediment core tops, but with a difference in the intercept with the Y-axis. This difference seems mainly determined by the low amount of crenarchaeol isomer VI (Fig. 1) in the incubation series. Recent ^{13}C NMR analysis of this compound indicates that compound VI is a regio-isomer of crenarchaeol. Interestingly, regio-isomers of GDGTs II-V have also been observed in increasing amounts with increasing temperature in the samples from sediment cores. It seems however, that this regio-isomer adaptation for membrane fluidity is less strong in the species present in our North Sea incubations than in tropical Crenarchaeota.

Thus, the calibrations carried out in our culture experiments have confirmed the usefulness of the TEX_{86} as a new proxy for the reconstruction of sea-surface temperatures of the earths' history.