Data repository on procedures for organic geochemical and isotopic analyses

Dried and homogenized sediments (~1.5 g dry mass) were extracted with dichloromethane (DCM)/methanol (2:1) by using the Dionex accelerated solvent extraction technique. The extracts were separated by Al₂O₃ column chromatography using hexane/DCM (9:1), DCM/methanol (95:5), and DCM/methanol (1:1) as subsequent eluents to yield the apolar, glycerol dialkyl glycerol tetraether (GDGT) and polar fractions, respectively. The apolar fractions were analysed by gas chromatography (GC) and GC-mass spectrometry. Prior to analyses by GC-isotope ratio monitoring spectrometry, the apolar fraction was separated with an AgNO₃ column using hexane and DCM to yield the aliphatic and the non-aliphatic fractions, respectively. Perdeuterated C_{20} and C_{24} *n*-alkanes were coinjected to monitor analytical precision (0.2 ‰ and 0.3 ‰, respectively). GDGT fractions were analyzed according to Schouten et al. (2007). Single ion monitoring of the [M + H] + ions (dwell time, 234 ms) was used to quantify the GDGTs with 1-4 cyclopentyl moieties (Schouten et al., 2007) and calculate the TEX₈₆ values. These values were converted to SST according to the equation $TEX_{86} = 0.027$ * SST -0.016 (Schouten et al., 2003) based on correlating TEX₈₆ values of Holocene coretop sediments with annual mean SSTs ranging between 20 and 28 °C. Above 28 °C we used the linear correlation line labeled B in fig. 2 of Schouten et al. (2003) as an extrapolation for the temperature range. Replicate analyses indicated that the analytical error in TEX_{86} values is 0.01, corresponding to a precision of SST for the samples of this study of ca. 0.6 °C.

The Carbon Preference Index (CPI), a measure of thermal maturity and dominance of terrigenous organic matter using nC₂₄ to nC₃₂ n-alkanes (Bray and Evans, 1961), was calculated to support the discussion on sources of organic matter.

References

Bray, E.E., and Evans, E.D., 1961, Distribution of n-paraffins as a clue to recognition of source beds: Geochimica et Cosmochimica Acta, v. 22, p. 2-15.

- Schouten, S., Hopmans, E.C., Forster, A., van Breugel, Y., Kuypers, M.M.M., and Damste, J.S.S., 2003, Extremly high sea-surface temperatures at low latitudes during the middle Cretaceous as revealed by archaeal membrane lipids: Geology, v. 31, p. 1069-1072.
- Schouten, S., Huguet, C., Hopmans, E.C., and Sinninghe Damsé, J.S., 2007, Improved analytical methodology of the TEX₈₆ paleothermometry by high performance liquid chromatography/atmospheric pressure chemical ionization-mass spectrometry:

 Analytical Chemistry, v. 79, p. 2940-2944.