Supplement of

Performance of temperature and productivity proxies based on long-chain alkane-1, mid-chain diols at test: a 5-year sediment trap record from the Mauritanian upwelling

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Supplemental Figures:

Supplemental Figure S1: Demonstration of the logarithmic nature of the diol flux data and the extraordinary effect of a single extreme on the regression line through the untransformed data in contrast to the minor effect of such an extreme on the log transformed data. Solid red line with outlier (red filled dot). Dashed blue line regression without outlier (blue open circles only).
Supplemental Figure S2: Regressions of natural logarithms of the diol flux data prior to and after correction. Solid green, for CBeu1-4, open red, for CBeu5. The four plots in the upper right corner provide examples prior to correction and demonstrate how the log normalized flux data for CBeu1-4 are systematically lower than and do hardly overlap with those of CBeu5. The remaining plots represent how the datasets agree after multiplying the fluxes of CBeu1-4 by 21.71.
Supplemental Figure S3: Upper panel, green dashed line with empty circles, initial values for CBeu5, red with filled circles final record with initial values for CBeu1–4 and after subtraction of 0.094 $U'_{K'}$ units from the CBeu5 record. Black line satellite-derived SST values ($SST_{UK}$) shifted by 35 days. Clearly visible is that the global calibration accurately reconstructs $SST_{UK}$ for CBeu1–4 and that the $SST_{UK}$ values for CBeu5 are shifted upwards relative to this $SST_{UK}$. SST values for March 2007–March 2008 are on average 0.6°C lower compared to March 2003–March 2007, the uncorrected $U'_{K'}$ do follow this trend for the last four samples of CBeu4 but at the transition to CBeu5 they increase and are on average 1.3°C higher than the preceding years. Since for CBeu1–4 the $SST_{UK}$ accurately reconstructs $SST_{UK}$, and since the offset occurs at the transition from one dataset (CBeu1–4 by Mollenhauer et al., 2014) to the other (CBeu5 new data), we consider the offset to be of analytical origin and applied a correction.

Lower 6 smaller panels. Regressions for CBeu1–4 (blue solid dots), CBeu 5 (red empty dots) and CBeu1–5 (lowermost three panels, orange). Top left and top middle, regression lines of $U'_{K'}$ to $SST_{UK}$ using the phase with the highest correlation. Green - line, global calibration line for suspended particulate matter (SPM) of Conte et al. (2006). Other panels, fit of reconstructed ($SST_{UK}$) temperatures to $SST_{UK}$ with green line x=y. Left panels without correction for CBeu5, middle panels, using the Conte et al., 2006 calibration, right panels, using the local cubic calibration.
Supplemental Figure S4: Fluxes of LDI diols (relative to total flux) sorted in order of decreasing flux with the sample having the highest flux rank number 1 and the sample with lowest flux rank number 83. On average the flux decreases by 6.7% each successive sample so that it is reduced by 50% every 10 samples.

\[ y = 23.1 \ln(x) + 0.338 \]

\[ R^2 = 0.99 \]
Supplemental Figure S5: Cumulative integrated production temperatures for SST\textsubscript{LDI} (IPT\textsubscript{LDI}, red triangles) and SST\textsubscript{SAT} (IPT\textsubscript{SAT}) with outliers (blue circles) and without outliers (green diamonds). Upper panels (a) samples in order of increasing flux; (b) samples in order of decreasing flux; Lower panels IPT\textsubscript{LDI} difference from IPT\textsubscript{SAT} in order of (c) increasing and (d) decreasing flux. The first value (rank 1) represents the IPT of the sample with the lowest (panels, a,b) or highest (panels, c,d) flux. In (a,b) the next value has the IPT of the next higher (a) or lower (b) sample added, and so on. The last value represents the IPT of the entire time series. The difference between the circles and diamonds clearly demonstrate the influence of outliers of intermediate flux. It is also clear that from sample 40 adding successively higher diol fluxes (a) results in successively higher IPT\textsubscript{LDI} and IPT\textsubscript{SAT} until the 20 samples with highest fluxes where this trend continues in the IPT\textsubscript{LDI} but ceases in the IPT\textsubscript{SAT}.