Supplements to

Microscale Alkenone Heterogeneity and Replicability of Ultra-High-Resolution Temperature Records from Marine Sediments

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S1 FT ICR MS settings

Table S1: Selected parameters for laser-desorption-ionization (LDI) FT-ICR-MS for compounds in the mass range around 554 m/z ("alkenone window")

Setting	Value
Q1 (m/z)	554 m/z
Q1range (m/z)	544-564
wordsize	512k
Detection mode	broadband
excitation mode	sweep
excitation range (m/z)	300-2000
shotraster	100µm
scans per shot	1
spot size	medium
laser power	varied according to sediment conditions
laser frequency	500 Hz
laser number of shots	250
Plate 1 final voltage for ramp 2	0.0 V
Plate 1 initial ramp voltage	1.0 V
Plate 1 final voltage for ramp 1	0.6 V
Gated Injection DC Bias 0	3.6 V
Internal Filament Current [Instrument Param]	0.500 A
Plate 2 initial ramp voltage	1.0 V
Plate 2 final voltage for ramp 1	0.6 V
Plate 2 final voltage for ramp 2	0.0 V
Gated Injection DC Bias 180	2.4 V

Front Trap Plate	3.0 V
Back Trap Plate	3.0 V
Internal Ionization Energy	1.0 eV
Gated Injection DC Bias 90	2.7 V
Back Trap Plate Quench	-30.0 V
Sidekick	0.0 V
Shimming DC Bias 90	3.0 V
Shimming DC Bias 270	3.0 V
Shimming DC Bias 0	3.0 V
Shimming DC Bias 180	3.0 V
ECD Lens	10.0 V
Gated Injection DC Bias 270	3.3 V
Analyzer Entrance	-10.0 V
Sidekick Offset	-1.5 V
Octopole 2 DC [Instrument Param]	2.0 V
Octopole Frequency	1
Extract [Instrument Param]	-10.0 V
Trap [Instrument Param]	10.0 V
Octopole 1 DC Bias (Low) [Instrument Param]	3.5 V
Octopole 2 DC Bias (High)	2.5 V
Octopole RF Amplitude	350.0 Vpp
Partition Lens [Instrument Param]	3.0 V
Octopole 2 Delta DC	0.0 V

S2 Time series summary

Table S2: Time-series data and row-wise averages across replicates per depth interval. Standard errors below 0.001 (~0.03°C) are not shown.

Depth (cm)	Mean	Variance	Average variance of swUK per horizon	Average number of successful detections of both alkenones per horizon	Average number of successful detections of any alkenone per horizon
0-5	0.523	0.00044	0.006	34.2 ± 1.6	38.6 ± 1.8

5-10	0.536 ± 0.001	0.000412	0.0059	42.2 ± 0.8	48.1 ± 0.9
10-15	0.543	0.000611	0.006	16 ± 0.8	19.2 ± 0.9
15-20	0.539 ± 0.001	0.000388	0.0062	24.8 ± 1	31.4 ± 1.1
20-25	0.538 ± 0.001	0.000898	0.0061	32.2 ± 3.8	38.4 ± 4.4
25-30	0.530 ± 0.001	0.000994	0.0059	39 ± 1.9	46.3 ± 1.7

S3 Xray Image Correction

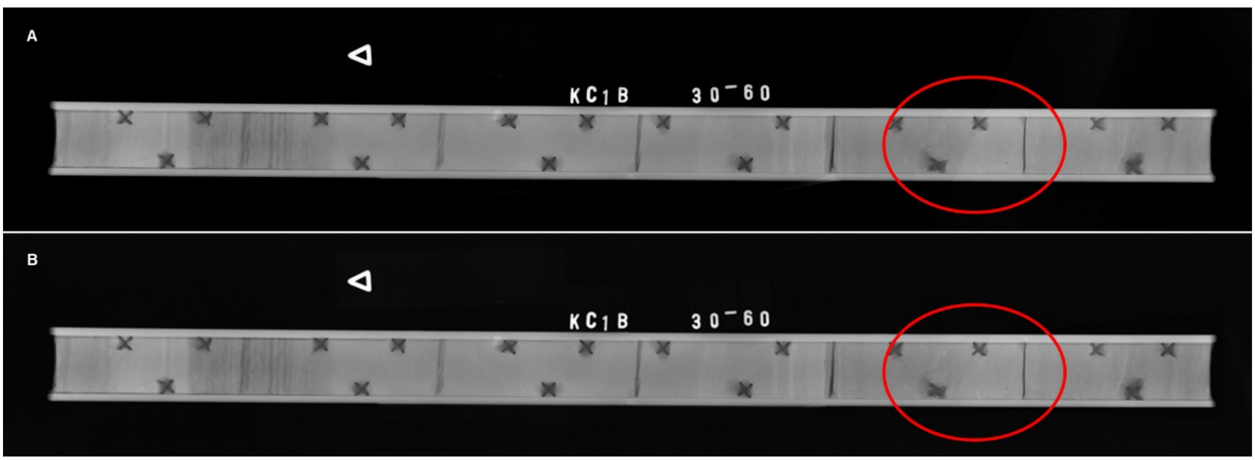

Figure S3: Comparison of the unaltered and corrected X-ray density maps for sediment segment KC1. Section 20-25 cm had an exposure artefact after developing, which was corrected digitally using Adobe Photoshop (2024).

S4 Individual variograms per depth

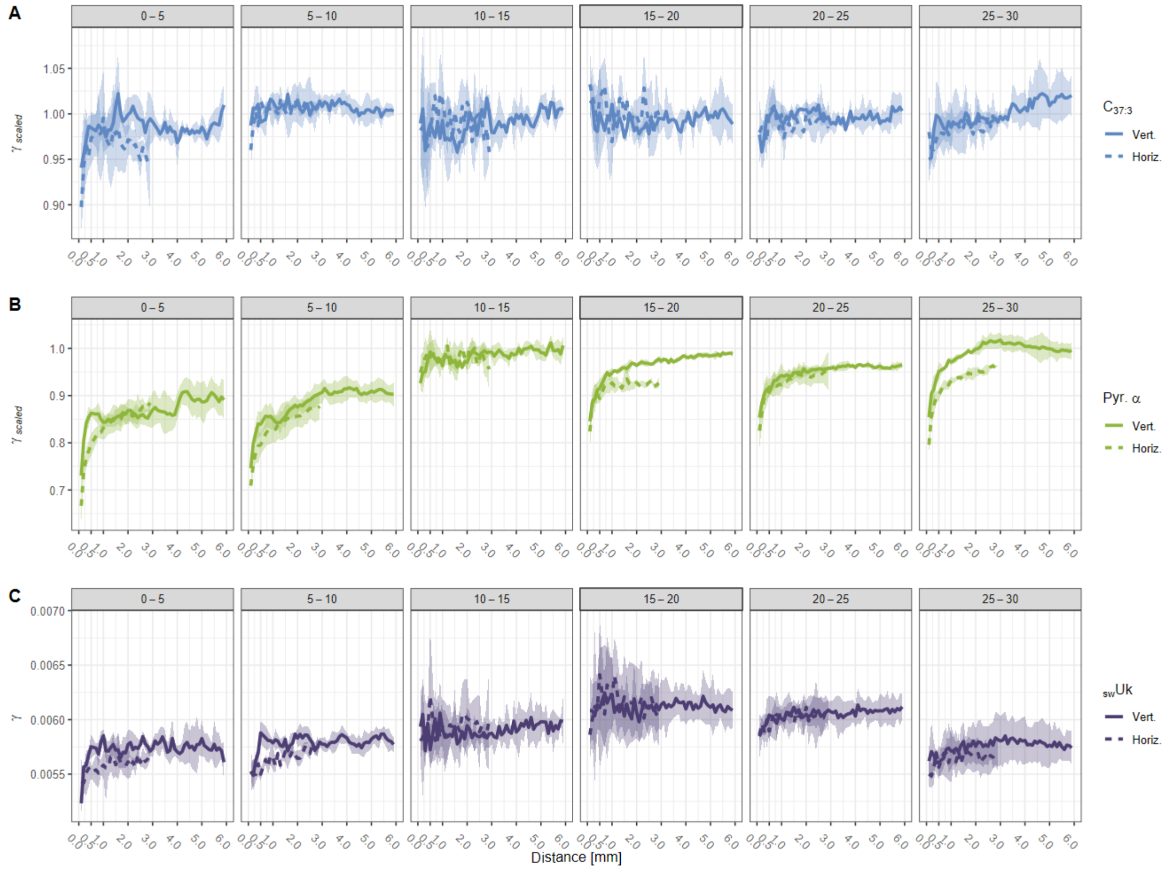

Figure S4: Variogram estimates averaged per depth interval of sediment segment KC1 for C37:3 and pyropheophorbide α intensities and spotwise Uk'37 temperatures. Note that each row has individual y-axes. C37:3 and pyropheophorbide α values in A, B were scaled prior calculation and are not in their native units, whereas in C γ values correspond to spotwise $U^{K'}_{37}$ units.

S5 Comparison to SST

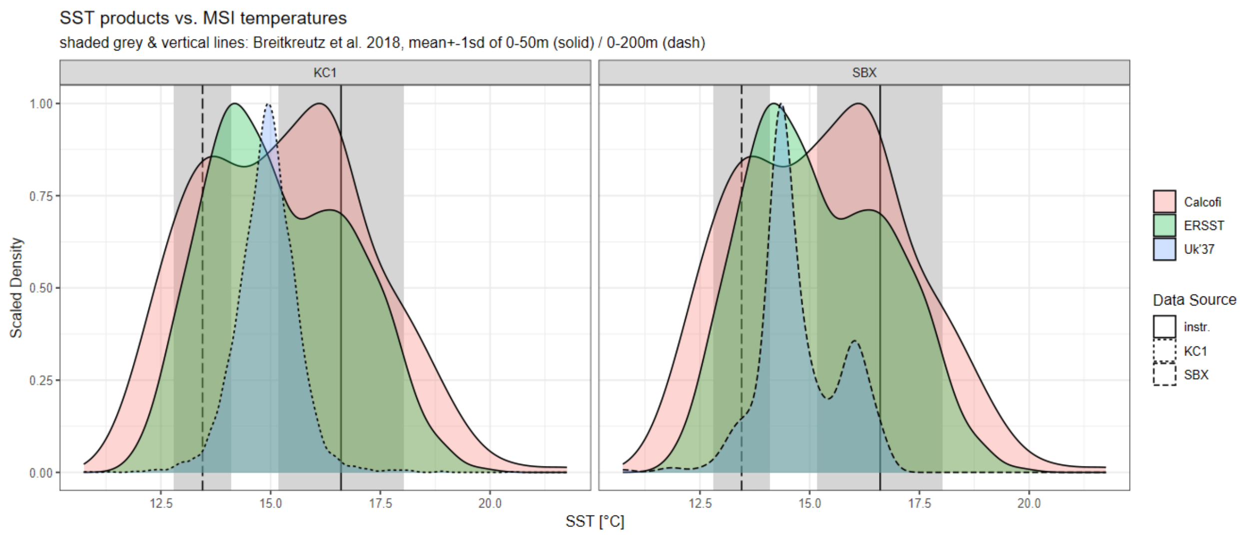

Figure S5: Comparison of MSI-derived SST estimates and SST products. Sediment data from KC1 segment, and the SBX 20-25cm exemplary varved section from Alfken et al. 2020, both converted to temperature using ISU and MSW approaches and the Prahl & Wakeham (1987) calibration ($U_{37}^{K'} = 0.033T + 0.043$). External SST data from the nearest location in Breitkreutz et al. (2018) (Lon: -119.5, Lat: 33.5) shown as vertical lines and shaded grey area (mean+-1sd of 0-50m and 0-200m respectively); ERSSTv4 (Huang et al., 2015) at Lon: 120, Lat: 34); and the nearest CalCOFI station (81.8-46.9) temperatures integrated 0-30m over 1984-2009 (California State Department of Fish and Game; NOAA Fisheries; Scripps Institution of Oceanography, 2001) (accessed 03/03/2023).

References

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