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Supplement of

Assessing the potential of amino acid ^{13}C patterns as a carbon source tracer in marine sediments: effects of algal growth conditions and sedimentary diagenesis

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Figure S1. GC-C-IRMS trace of amino acid derivatives from sediment sample “sed689” purified with Bio-Rad’s 50W-X8 100–200 mesh resin prior to derivatization. The amino acids were derivatized to N-acetyl methyl esters and separated on a Thermo TraceGOLD TG-200MS GC column (60 m x 0.32 mm x 0.25 μ m) on a Agilent 6890N GC connected with a MAT 253 isotope ratio mass spectrometer (IRMS) via a GC-III combustion (C) interface (Thermo-Finnigan Corporation).

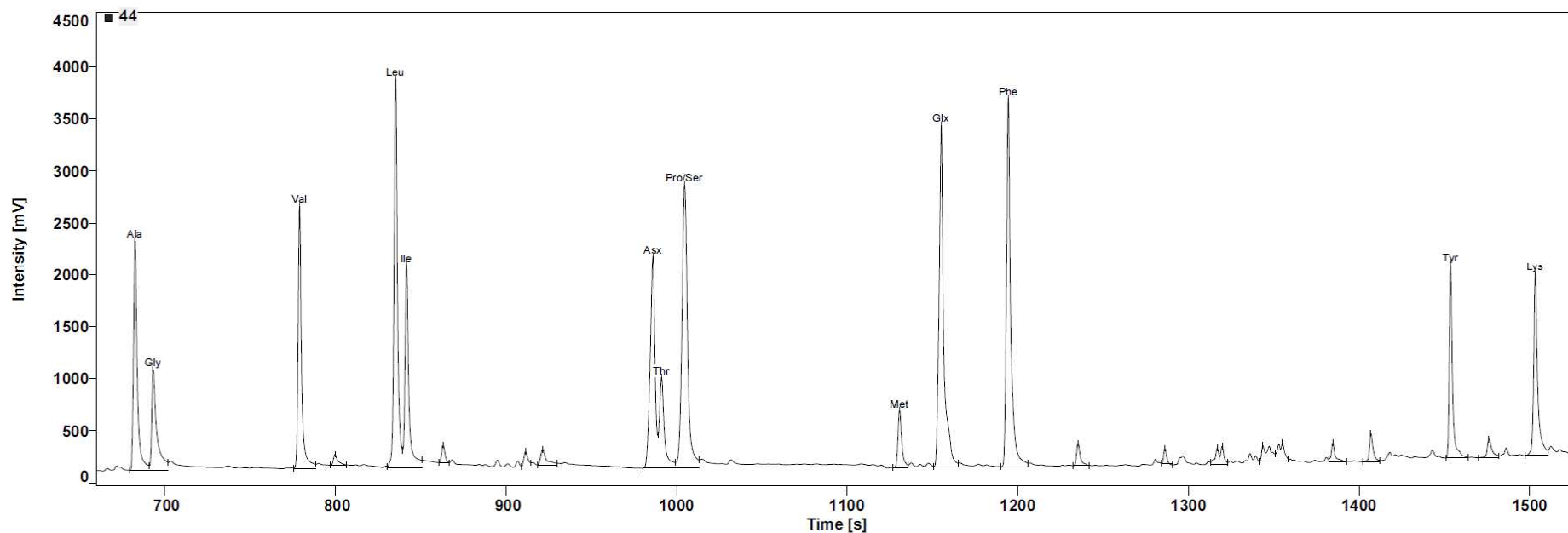


Figure S2. The effect of Bio-Rad’s 50W-X8 100–200 mesh resin sample purification on amino acid $\delta^{13}\text{C}$ values. The test was performed on yeast samples and a mixture of amino acid standards, respectively. For the yeast samples, we used acid hydrolyzed freeze-dried material (each yeast samples comprised of 2.5 mg DW yeast hydrolyzed in 6N HCl at 110°C for 20 h). The standards were obtained from pure amino acids dissolved in a 0.1 N HCl solution. Before purification, the samples were dried and redissolved in 4 ml 0.05 M HCl. The unfilled boxplots represent the control treatments and the filled boxplots the purified samples (3 replicate samples with each replicate representing the mean isotope value of 3 sample injections). Single asterisk (*) represents significant of the 0.05 level and “ns” signifies non-significant differences ($P > 0.05$).

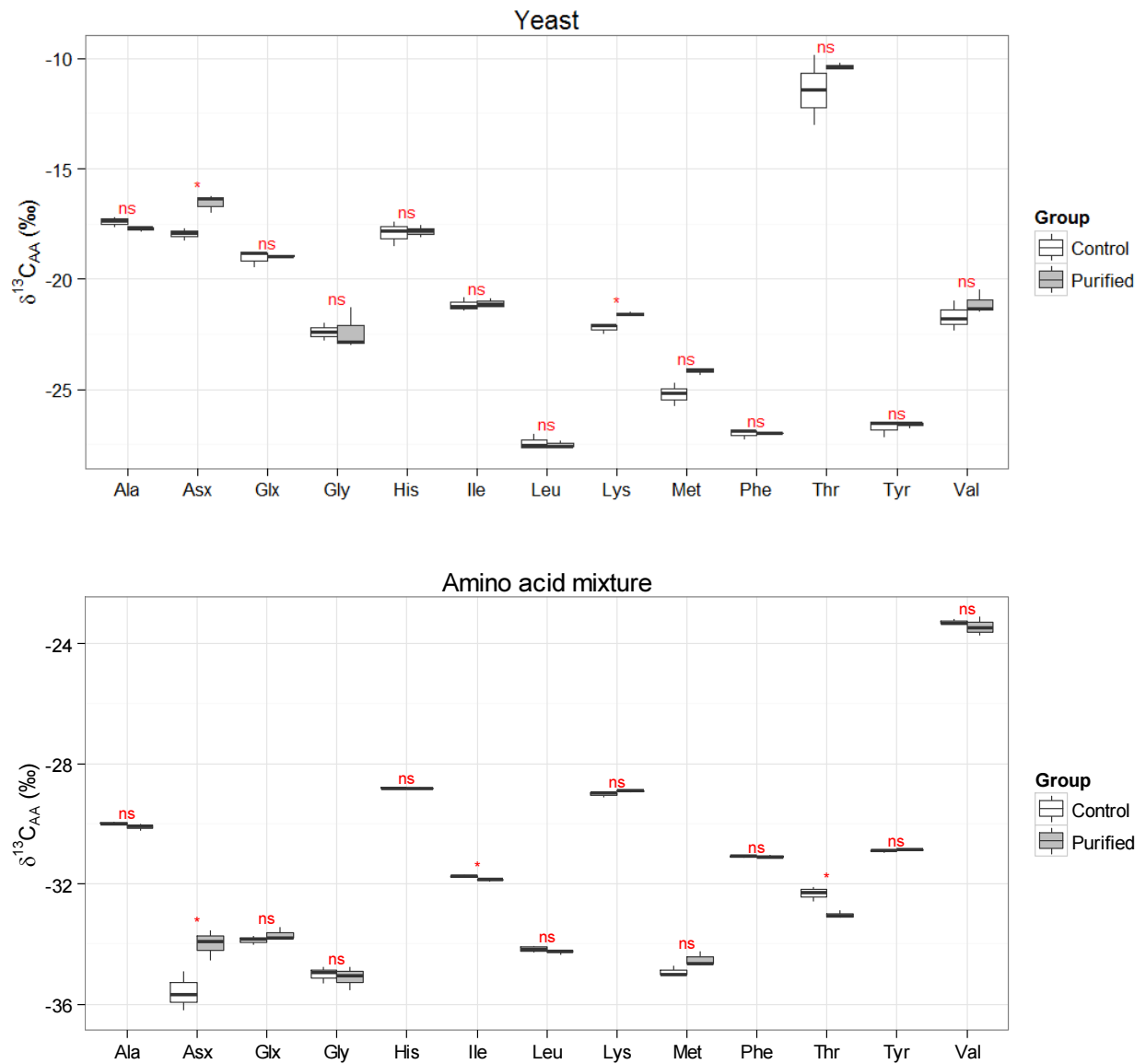
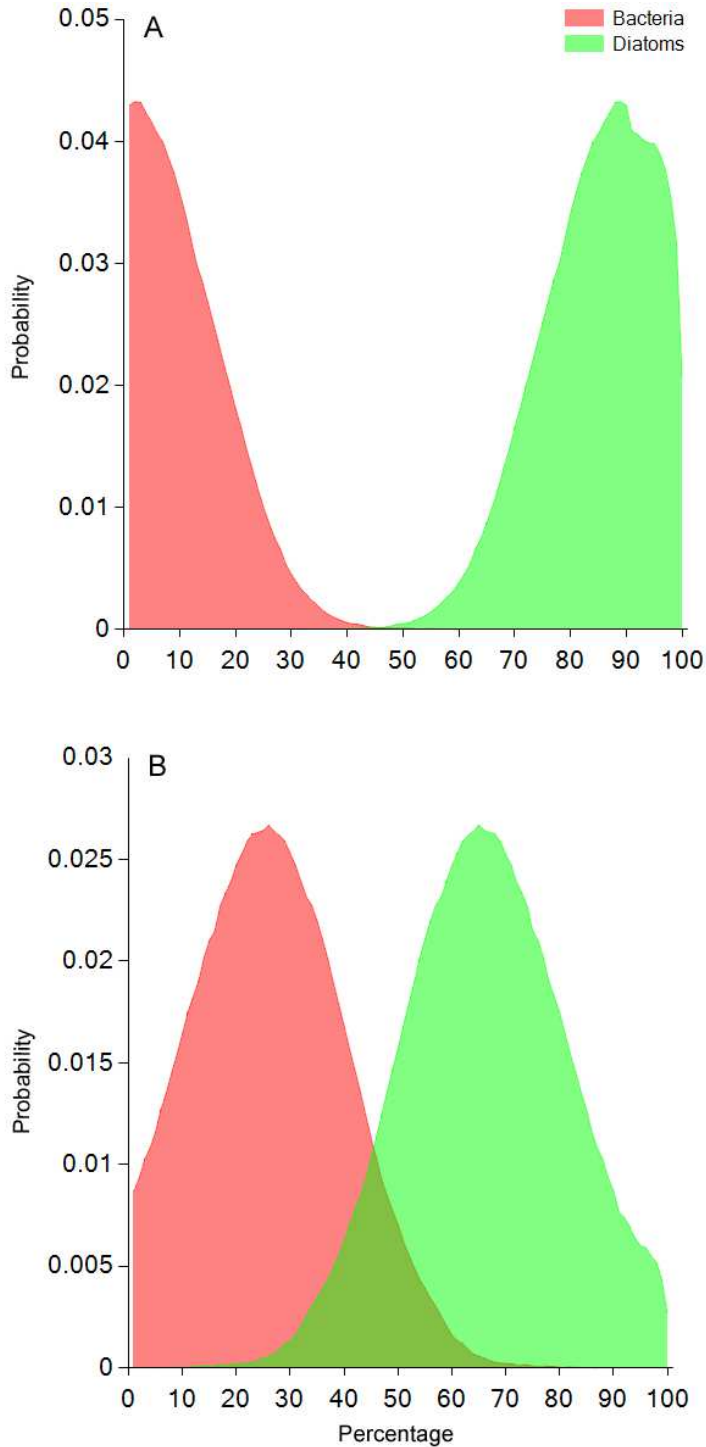


Figure S3. Probability distribution of bacterial and diatom origins of amino acids in two sediment layers, 8 cm (A) and 998 cm (B) of core M772-003-2 from the Peruvian margin. The Bayesian mixing modeling output is based on normalized $\delta^{13}\text{C}$ values of leucine, lysine, isoleucine and tyrosine.



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Table S1. Amino acid $\delta^{13}\text{C}$ values of *Thalassiosira weissflogii* of ten different treatments. The isotope values represent the means and standard deviations of each sample (n). The average analytical standard deviations (SD) across all samples are shown in the lowermost row. See Table 1 in the main text for description of sample identities.

Treatment	n	Thr	Asx	Lys	Ile	Met	Ala	Val	Leu	Arg	Glx	Tyr	Phe
Ctrl	a	-11.6± 0.2	-15.9±0.3	-18.9± 0.3	-21.7±0.1	-21.1±0.2	-18.0±0.1	-28.8±0.0	-31.3±0.2	-22.8±1.5	-23.3±0.1	-25.8±0.3	-29.6±0.1
Ctrl	b	-11.4± 0.0	-16.4±0.0	-20.4± 0.8	-21.9±0.1	-21.5±0.1	-17.7±0.1	-28.1±0.1	-31.4±0.3	-22.2±0.8	-23.0±0.1	-26.2±0.2	-29.7±0.1
Ctrl	c	-11.2± 0.3	-15.3±0.1	-19.4± 0.4	-21.2±0.1	-21.1±0.3	-17.3±0.1	-28.2±0.1	-31.1±0.2	-21.2±0.2	-23.2±0.1	-25.8±0.2	-29.5±0.0
Irr.H	a	-12.0± 0.5	-16.5±0.1	-20.0± 0.4	-22.5±0.3	-22.1±0.4	-18.5±0.4	-29.5±0.1	-32.0±0.3	-22.5±1.1	-23.9±0.2	-26.1±0.2	-29.7±0.2
Irr.H	b	-13.6± 0.5	-15.3±0.7	-19.4± 0.2	-22.4±0.2	-21.8±0.0	-17.8±0.3	-29.4±0.1	-32.1±0.5	-21.1±0.2	-23.8±0.1	-26.4±0.2	-30.1±0.2
Irr.L	a	-10.7± 0.4	-18.4±0.1	-18.2± 0.2	-21.0±0.1	-20.4±0.2	-15.9±0.5	-28.8±0.2	-31.8±0.1	-21.1±0.7	-22.3±0.1	-25.7±0.1	-29.5±0.1
Irr.L	b	NA	NA	-18.2± 0.3	NA	-20.6±0.2	NA	NA	NA	-22.8±0.5	-23.0±0.1	-26.3±0.1	-29.9±0.3
Irr.L	c	NA	NA	-18.3± 0.1	NA	-20.4±0.2	NA	NA	NA	-22.4±0.4	-22.8±0.2	-26.1±0.2	-29.7±0.0
pH.H	a	-7.6± 0.2	-14.0±1.8	-14.4± 0.2	-17.8±0.1	-16.9±0.8	-13.9±0.5	-26.0±0.1	-27.7±0.2	-18.7±0.8	-19.1±0.3	-22.3±0.2	-26.0±0.2
pH.H	b	-11.8± 0.4	-11.7±0.5	-15.3± 0.0	-17.5±0.7	-17.0±0.0	-13.9±0.5	-25.9±0.0	-27.8±0.7	-19.3±0.2	-19.0±0.5	-22.4±0.1	-26.3±0.0
pH.H	c	-12.6± 0.5	-12.0±1.0	-15.5± 0.4	-17.9±0.0	-17.5±0.2	-13.7±0.2	-25.8±0.2	-27.7±0.1	-18.7±0.6	-19.3±0.1	-22.6±0.1	-26.4±0.0
pH.L	a	-10.9± 0.3	-17.7±2.5	-20.2± 0.3	-21.5±0.1	-21.9±0.4	-17.5±0.3	-29.2±0.2	-32.1±0.2	-22.5±0.4	-23.8±0.2	-26.6±0.1	-30.2±0.2
pH.L	b	-11.2± 0.1	-18.6±2.5	-19.4± 0.7	-21.8±0.1	-21.3±0.1	-18.3±0.4	-29.3±0.1	-32.0±0.2	-22.3±0.9	-23.7±0.1	-26.4±0.3	-30.1±0.2
pH.L	c	-9.5± 2.3	-18.1±2.3	-19.2± 0.9	-21.8±0.2	-21.7±0.3	-18.8±0.3	-29.3±0.1	-32.2±0.1	-22.8±0.5	-23.8±0.1	-26.2±0.2	-30.1±0.1
Psu.L	a	-12.6± 0.2	-20.1±0.0	-23.0± 0.8	-25.0±0.1	-25.0±0.2	-20.2±0.4	-33.9±0.2	-35.6±0.1	-23.8±2.4	-27.3±0.2	-30.0±0.3	-34.1±0.2
Psu.L	b	-13.8± 0.0	-21.9±1.1	-23.4± 0.5	-26.3±0.2	-25.4±0.6	-21.4±0.2	-35.2±0.4	-36.6±0.2	-26.1±0.2	-28.5±0.2	-31.2±0.2	-35.2±0.1
Psu.L	c	-13.9± 2.1	-21.5±0.1	-24.6± 0.7	-26.8±0.2	-25.6±1.0	-22.2±0.3	-35.5±0.2	-36.9±0.2	-25.5±0.4	-28.5±0.2	-31.4±0.1	-35.3±0.3
T.18	a	-4.0± 1.8	-12.1±1.9	-14.7± 0.5	-16.9±0.1	-16.0±0.4	-12.3±0.3	-26.6±0.1	-27.5±0.0	-18.4±1.5	-18.6±0.1	-22.4±0.3	-25.5±0.1
T.18	b	-5.4± 0.2	-11.9±1.3	-15.2± 0.5	-16.6±0.2	-16.6±0.8	-12.5±0.3	-23.5±0.2	-27.6±0.2	-19.5±1.5	-18.8±0.1	-22.5±0.3	-25.5±0.2
T.18	c	-3.7± 1.5	-11.6±1.2	-14.7± 0.5	-16.8±0.2	-16.1±0.9	-12.5±0.3	-24.2±0.2	-27.7±0.2	-18.9±1.2	-18.9±0.2	-22.3±0.5	-25.7±0.2
T.27	a	-4.8± 0.1	-11.9±2.0	-14.1± 0.3	-15.1±0.1	NA	-10.8±0.1	-23.6±0.1	-25.3±0.0	-17.2±0.7	-16.6±0.2	-21.9±0.3	-24.3±0.1
T.27	b	-4.8± 0.5	-10.6±0.2	-13.3± 0.4	-15.5±0.1	NA	-10.9±0.1	-25.3±0.1	-25.8±0.1	-16.6±0.8	-17.0±0.2	-22.1±0.3	-24.9±0.1
T.27	c	-4.6± 0.4	-10.6±1.0	-15.2± 0.4	-15.9±0.2	-14.6±0.6	-11.6±0.1	-25.3±0.1	-26.2±0.1	-17.7±1.6	-17.5±0.1	-22.5±0.3	-25.2±0.2
UV.ct	a	-12.9± 0.4	-16.7±2.2	-17.8± 0.2	-20.1±0.1	-20.2±0.1	-15.7±0.2	-28.5±0.1	-30.7±0.4	NA	-23.1±0.0	-26.0±0.0	-29.4±0.1
UV.ct	b	-10.2± 0.2	-16.2±2.7	-17.3± 0.3	-19.6±0.1	-19.5±0.4	-15.5±0.2	-28.2±0.1	-30.1±0.3	-22.0±0.9	-22.6±0.1	-25.3±0.1	-28.9±0.1
UV.ct	c	-11.2± 0.5	-15.5±0.4	-18.4± 0.3	-20.2±0.0	-19.8±0.1	-16.5±0.1	-28.9±0.0	-30.5±0.1	-21.4±0.2	-23.1±0.1	-25.9±0.2	-29.2±0.1
UV.tr	a	-11.8± 0.5	-17.0±2.5	-18.1± 0.2	-20.0±0.0	-19.7±0.2	-16.0±0.3	-28.7±0.0	-30.4±0.1	NA	-23.1±0.1	-25.7±0.1	-29.1±0.1
UV.tr	c	-9.3± 0.1	-15.7±0.3	-19.7± 0.4	-20.7±0.1	-20.5±0.1	-17.1±0.3	-29.5±0.1	-31.1±0.3	-20.0±0.3	-23.7±0.0	-25.9±0.2	-30.0±0.1
SD mean		0.6	1.1	0.4	0.1	0.3	0.2	0.1	0.2	0.8	0.1	0.2	0.1

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Table S2. Amino acid $\delta^{13}\text{C}$ values (in ‰) of diatoms, bacteria and core M772-003-2 samples. The isotope values represent the means and standard deviations of each sample (n). The average analytical standard deviations (SD) across all samples are shown in the lowermost row. Bacteria species: B1; *Burkholderia xenovorans*, B2; *Methylobacterium* sp, B3; *Klebsiella* sp, B4; *Rhodococcus* spp., B5-B12; Unidentified species. Diatom species: D1; *Achnanthes brevipes*, D2; *Amphora coffaeiformis*, D3; *Melosira varians*, D4; *Phaeodactylum tricornutum*, D5-D6; *Stauroneis constricta*, D7; *Thalassiosira weissflogii*, N1-N3: Assemblage of diatom species from Kiel Fjord. See Table 3 in the main text for description of sediment samples. The asterisk symbol (*) denotes that the $\delta^{13}\text{C}$ values were obtained from Larsen et al. (2013).

ID	Ala	Asx	Glx	Gly	His	Ile	Leu	Lys	Met	Phe	Thr	Tyr	Val
Bacteria													
B1*	-11.3± 0.1	-12.9± 0.9	-11.5± 0.0	-12.9± 0.1	-8.4± 0.9	-12.0± 0.0	-12.8± 0.1	-10.4± 0.1	-18.6± 0.1	-18.8± 0.0	-5.2± 0.8	-16.8± 0.1	-13.6± 0.1
B2*	-12.2± 0.0	-17.6± 0.3	-17.8± 0.0	-13.9± 0.0	-8.1± 0.7	-12.9± 0.1	-13.0± 0.0	-14.9± 0.1	-18.5± 0.2	-17.0± 0.1	-8.2± 1.4	-18.1± 0.1	-14.1± 0.1
B3*	-15.9± 0.0	-21.8± 0.7	-18.3± 0.0	-21.3± 0.2	-16.0± 0.4	-18.9± 0.2	-19.9± 0.0	-20.3± 0.2	-25.7± 0.3	-24.6± 0.1	-15.0± 0.8	-22.9± 0.0	-20.8± 0.0
B4*	-22.6± 0.0	-22.7± 0.4	-22.9± 0.0	-25.3± 0.1	-22.2± 0.4	-23.7± 0.1	-25.2± 0.2	-21.2± 1.1	-27.5± 0.2	-28.9± 0.1	-15.1± 0.1	-27.7± 0.2	-26.4± 0.2
B5*	-14.8± 0.1	-17.4± 0.6	-16.5± 0.0	-13.8± 0.4	-8.1± 0.2	-16.1± 0.1	-17.7± 0.3	-14.8± 0.2	-20.0± 0.2	-18.3± 0.1	-8.3± 0.2	-18.0± 0.0	-17.8± 0.1
B6*	-18.3± 0.1	-15.1± 0.1	-14.3± 0.1	-18.5± 0.1	-11.8± 0.2	-17.1± 0.5	-19.2± 0.1	-15.3± 0.1	-18.8± 0.2	-20.1± 0.1	-8.6± 1.3	-20.2± 0.1	-21.1± 0.0
B7*	-15.3± 0.0	-15.3± 0.9	-13.9± 0.0	-14.3± 0.1	-9.8± 0.0	-15.6± 0.2	-17.4± 0.1	-12.9± 0.2	-18.5± 0.1	-18.5± 0.1	-7.4± 0.3	-18.3± 0.1	-19.0± 0.0
B8*	-14.1± 0.1	-15.4± 0.7	-15.2± 0.0	-14.0± 0.3	-7.8± 0.3	-16.1± 0.2	-15.9± 0.0	-14.4± 0.1	-20.7± 0.3	-17.7± 0.0	-7.8± 0.5	-17.4± 0.2	-17.7± 0.0
B9*	-18.1± 0.1	-24.2± 0.9	-21.2± 0.0	-21.7± 0.2	-16.8± 0.2	-21.2± 0.5	-24.1± 0.5	-21.5± 0.1	-27.4± 0.3	-27.0± 0.0	-16.8± 0.2	-25.2± 0.1	-25.1± 0.1
B10*	-16.5± 0.0	-19.2± 0.0	-16.8± 0.1	-15.5± 0.3	-10.6± 0.4	-18.6± 0.1	-17.4± 0.1	-17.8± 0.2	NA	-20.9± 0.0	-12.2± 0.3	-19.7± 0.1	-21.4± 0.0
B11*	-17.2± 0.1	-18.9± 0.1	-18.5± 0.0	-16.9± 0.6	-11.8± 0.5	-18.6± 0.1	-19.0± 0.1	-18.5± 0.1	NA	-21.9± 0.1	-11.6± 0.7	-20.9± 0.1	-22.1± 0.1
B12*	-20.8± 0.1	-24.4± 0.0	-24.1± 0.0	-22.4± 0.4	NA	-24.0± 0.1	-24.2± 0.1	-24.8± 0.2	-31.6± 0.3	-28.7± 0.1	-17.9± 1.6	-25.5± 0.0	-26.0± 0.1
Microalgae													
D1*	-9.7± 0.1	-11.1± 0.4	-11.4± 0.1	-11.2± 0.2	NA	-10.2± 0.1	-17.3± 0.2	-8.8± 0.5	NA	-18.1± 0.3	-2.7± 0.8	-15.7± 0.1	-13.8± 0.1
D2*	-7.4± 0.2	-9.1± 0.3	-7.5± 0.0	-12.0± 0.4	NA	-11.5± 0.1	-18.7± 0.0	-11.1± 0.2	NA	-19.6± 0.2	-2.0± 0.9	-16.0± 0.1	-16.8± 0.2
D3*	-10.3± 0.2	-16.2± 0.2	-12.2± 0.1	-12.3± 0.6	NA	-16.5± 0.2	-22.1± 0.1	-15.8± 0.0	-15.0± 0.5	-20.6± 0.3	-7.0± 0.1	-19.4± 0.1	-19.7± 0.1
D4*	-16.0± 0.5	-17.7± 0.7	-18.9± 0.1	-12.2± 0.6	NA	-16.1± 1.3	-25.5± 0.3	-15.2± 0.3	NA	-23.8± 0.1	-10.8± 0.5	-21.8± 0.2	-22.9± 0.5
D5*	-1.3± 0.1	-6.6± 1.0	-7.4± 0.1	-5.5± 0.2	NA	-10.4± 0.1	-19.3± 0.1	-8.5± 0.2	-8.2± 0.4	-16.0± 0.4	-4.6± 0.5	-14.4± 0.2	-15.5± 0.1
D6	-4.2± 0.0	-4.2± 0.1	-7.5± 0.1	-6.2± 0.0	NA	-9.7± 0.6	-19.6± 0.0	-6.2± 0.1	NA	-16.5± 0.0	-3.1± 0.1	-14.6± 0.0	-16.2± 0.0
D7	-17.0± 0.1	-17.2± 0.3	-23.3± 0.1	-20.6± 0.2	NA	-21.0± 0.0	-31.6± 0.0	-18.5± 0.1	-21.3± 0.1	-29.3± 0.2	-11.3± 0.3	-26.2± 0.3	-29.1± 0.1
N1*	-17.4± 0.1	-18.9± 0.0	-20.3± 0.1	-21.7± 0.4	-19.2± 0.6	-21.0± 0.1	-29.7± 0.3	-18.1± 0.0	-21.7± 0.6	-27.0± 0.1	-11.0± 0.1	-24.8± 0.2	-26.4± 0.5
N2*	-17.4± 0.2	-18.2± 0.1	-20.3± 0.1	-21.9± 0.3	-20.8± 0.2	-20.6± 0.1	-29.3± 0.3	-18.0± 0.2	-19.2± 0.6	-26.8± 0.1	-11.2± 0.1	-24.5± 0.2	-27.2± 0.2
N3*	-17.4± 0.2	-17.8± 0.2	-20.4± 0.0	-21.8± 0.6	-21.5± 0.2	-19.8± 0.1	-29.4± 0.2	-17.9± 0.2	-21.2± 0.4	-26.9± 0.1	-10.7± 0.1	-24.7± 0.2	-27.1± 0.1
Peruvian sediment													
M772-8	-16.5± 0.5	-14.5± 0.3	-17± 0.1	-11.9± 0.2	-14.3± 0.4	-20.9± 0.1	-28.2± 0.9	-16.6± 0.1	-18.7± 0.4	-24.6± 0	-10.1± 0.2	-23.7± 0.4	-26.7± 0.5

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M772-13	-17.7 ± 0.2	-14.3 ± 0.3	-18.1 ± 0.1	-12.5 ± 0.3	NA	-21.3 ± 0.1	-28.4 ± 0.1	-17.2 ± 0.3	-18.5 ± 0.4	-24.9 ± 0.1	-10.9 ± 0.9	-23.7 ± 0.1	-26.5 ± 0.3
M772-268	-16.2 ± 0.5	-12.3 ± 0.5	-17.4 ± 0.1	-10.6 ± 0.6	NA	-18 ± 0.1	-26.7 ± 0.7	-15.0 ± 0.1	-17.9 ± 0.3	-23.5 ± 0.1	-10.0 ± 0.9	-22.5 ± 0.1	-23.8 ± 0.3
M772-278	-17.2 ± 0.3	-11.5 ± 0.5	-17.7 ± 0.1	-9.4 ± 0.3	-13.5 ± 0.1	-20.5 ± 0	-28.2 ± 0.2	-16.0 ± 0.1	-20.8 ± 0.2	-25.3 ± 0.1	-12.0 ± 0.2	-23.4 ± 0.2	-25.3 ± 0.2
M772-353	-17.7 ± 0.2	-15.7 ± 0.2	-18.1 ± 0.1	-12.4 ± 0.2	NA	-21.1 ± 0	-27.5 ± 0	-16.7 ± 0.2	-18.2 ± 0.4	-25.1 ± 0.1	-12.0 ± 1.0	-24.2 ± 0.1	-25.4 ± 0
M772-638	-17.6 ± 0.2	-8.9 ± 0.2	-18.3 ± 0.1	-9.13 ± 0.6	-14.1 ± 0.5	-21.6 ± 0.2	-26.8 ± 0.3	-16.2 ± 0.1	-20.3 ± 0.3	-25.3 ± 0.1	-11.4 ± 0.3	-23.7 ± 0.2	-25.4 ± 0.2
M772-689	-18.6 ± 0.2	-14.2 ± 0.2	-17.2 ± 0.3	-10.7 ± 0.3	NA	-19.7 ± 1.1	-25.3 ± 0.9	-15.3 ± 0.7	-18.4 ± 0.9	-23.6 ± 0.7	-10.3 ± 0.6	-22.8 ± 0.6	-25.2 ± 0.7
M772-998	-18.3 ± 0.1	NA	NA	-13.2 ± 0.1	NA	-22.0 ± 0.5	-27.2 ± 0.1	-18.1 ± 0.0	-20.2 ± 0.2	-25.4 ± 0.0	NA	-24.9 ± 0.2	-27.1 ± 0.2
M772-1023	-17.5 ± 0.3	-12.8 ± 0.4	-18.3 ± 0.3	-13.2 ± 0.2	NA	-22 ± 0.2	-27.5 ± 0.2	-17.7 ± 0.2	-19.9 ± 0.2	-24.9 ± 0.2	-10.5 ± 0.7	-23.8 ± 0.2	-26 ± 0.2
M772-1283	-17.1 ± 0.1	-13 ± 0.2	-21 ± 0.2	-12.4 ± 0.2	NA	-23.4 ± 0.1	-27.5 ± 0.1	-18 ± 0.1	-20.3 ± 0.6	-25 ± 0.1	-13.4 ± 0.2	-25.3 ± 0.1	-27.6 ± 0.1
M772-1413	-16.9 ± 0.4	-14.2 ± 0.7	-18.5 ± 0.1	-12.1 ± 0.2	NA	-21.8 ± 0.2	-27 ± 0.2	-17.6 ± 0.1	-19.7 ± 0.5	-24.9 ± 0.1	-10.7 ± 1.1	-24.3 ± 0.1	-26.8 ± 0.1

*Larsen, T., M. Ventura, N. Andersen, D. M. O'Brien, U. Piatkowski, and M. D. McCarthy. 2013. Tracing Carbon Sources through Aquatic and Terrestrial Food Webs Using Amino Acid Stable Isotope Fingerprinting. Plos One 8:e73441.

Supplement

Table S3. The estimated proportion of bacterial and diatom origins of amino acids in different sediment layers of core M772-003-2. Overall, the upper layers has less probability of bacterial amino acid contribution than the lower layers. The mixing model was based on the four most informative amino acids for distingusiing between bacteria and diatoms; Ile, Leu, Tyr, and Lys.

Sediment depth	Origins	Mean	Stdev	2.5pc	median	97.5pc
8	Bacteria	13.1	9.0	0.6	11.6	33.5
8	Diatoms	86.9	9.0	66.5	88.4	99.4
13	Bacteria	13.9	9.6	0.6	12.5	36.1
13	Diatoms	86.1	9.6	63.9	87.6	99.4
268	Bacteria	11.5	8.0	0.6	10.3	29.1
268	Diatoms	88.5	8.0	71.0	89.7	99.4
278	Bacteria	10.7	7.8	0.4	9.2	28.2
278	Diatoms	89.3	7.8	71.8	90.8	99.6
353	Bacteria	17.2	10.3	1.2	16.3	39.3
353	Diatoms	82.8	10.3	60.7	83.7	98.9
638	Bacteria	19.1	13.4	0.8	17.0	50.5
638	Diatoms	80.9	13.4	49.5	83.0	99.2
689	Bacteria	24.9	13.2	2.0	24.7	51.3
689	Diatoms	75.1	13.2	48.8	75.4	98.0
998	Bacteria	30.1	14.1	3.9	29.9	58.3
998	Diatoms	69.9	14.1	41.7	70.1	96.1
1023	Bacteria	24.3	13.9	1.7	23.4	53.5
1023	Diatoms	75.7	13.9	46.5	76.6	98.4
1283	Bacteria	34.9	20.5	2.4	33.0	81.7
1283	Diatoms	65.1	20.5	18.4	67.1	97.6
1413	Bacteria	29.7	15.1	3.3	29.2	60.2
1413	Diatoms	70.3	15.1	39.9	70.8	96.7