Supplementary Material

**Amino Acid δ13C and δ15N Fingerprinting of Sea ice and Pelagic Algae in Canadian Arctic and Subarctic Seas**

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**DOI**: 10.3389/fmars.2022.976908

1 Supplementary Discussion

## Effects of ultrasonication

To avoid contamination peaks introduced by hydrolyzing nylon filters, biomass was extracted from the nylon filters by ultrasonicating the filters in Milli-Q water at 40 kHz before hydrolysis. It is important to note that ultrasonic extraction may induce cell disruption which releases a portion of water-soluble proteins and free AAs (Rahman & Lamsal, 2021). The removal of the supernatant following the ultrasonication may lead to an overall smaller AA yield from the biomasses on the filters. While it is possible to selectively lose some AAs, the loss of AAs is unlikely to isotopically fractionate the AAs (Matthew D. McCarthy, personal communication, August 4, 2022). In fact, different AAs are subject to different degrees of losses during filtration through a peristaltic pump, acid hydrolysis and cation exchange clean-up, and yet minimal isotope fractionation was found despite the AA loss (Silverman et al., 2021). This is evidenced by the consistent δ13C-EAA and δ15N-SrcAA values of > 3 μm brash ice algae between the 2019 (non-ultrasonicated) and 2021 (ultrasonicated) collections (Fig. 2, 3). We found that the relative abundance (mol%) of amino acids were also consistent between different algal groups and size classes, suggesting the loss of AAs may play a minor role in affecting the isotopic values (Fig. S1). Nevertheless, it is important to acknowledge that this extra extraction step may pose challenges for future studies to replicate or compare with our findings.

2 Supplementary Tables and Figures

Table S Sampling locations and depth, size, and biomass analyzed of sea ice and pelagic algae samples.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample ID** | **Year** | **Location** | **Station** | **Algae type** | **Samples** | **Size (μm)** | **Depth (m)** | **Biomass (mg)** |
| IC1-H-Apr | 2017 | Cambridge Bay | CB | Sea ice | Fast ice | > 0.7 | NA | NA |
| IC1-H-May | 2017 | Cambridge Bay | CB | Sea ice | Fast ice | > 0.7 | NA | NA |
| IC2-L-Apr | 2017 | Cambridge Bay | CB | Sea ice | Fast ice | > 0.7 | NA | NA |
| IC2-L-May | 2017 | Cambridge Bay | CB | Sea ice | Fast ice | > 0.7 | NA | NA |
| IC4-L-Apr | 2017 | Cambridge Bay | CB | Sea ice | Fast ice | > 0.7 | NA | NA |
| IC4-L-May | 2017 | Cambridge Bay | CB | Sea ice | Fast ice | > 0.7 | NA | NA |
| ICEn1a | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | > 3 | 0 | 4.8 |
| ICEn1b | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | > 3 | 0 | 4.8 |
| ICEn2a | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | > 3 | 0 | 7.6 |
| ICEn2b | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | > 3 | 0 | 7.6 |
| ICEn3a | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | > 3 | 0 | 14.9 |
| ICEn3b | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | > 3 | 0 | 14.9 |
| ICEp1 | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | 0.2-3 | 0 | 2.2 |
| ICEp2 | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | 0.2-3 | 0 | 2.5 |
| ICEp3 | 2019 | Frobisher Bay | FB | Sea ice | Brash ice | 0.2-3 | 0 | 3.9 |
| 1-15-0-N | 2019 | Labrador Shelf | IC | Pelagic | Seawater | > 3 | 0 | 11.7 |
| 1-15-1-N | 2019 | Labrador Shelf | IC | Pelagic | Seawater | > 3 | 30 | 9.1 |
| 1-15-0.5-P | 2019 | Labrador Shelf | IC | Pelagic | Seawater | 0.2-3 | 15 | 5.1 |
| 1-15-0-P | 2019 | Labrador Shelf | IC | Pelagic | Seawater | 0.2-3 | 0 | 1.9 |
| 1-15-1-P | 2019 | Labrador Shelf | IC | Pelagic | Seawater | 0.2-3 | 30 | 3.4 |
| NS3-0.5-N | 2019 | Labrador Shelf | NS | Pelagic | Seawater | > 3 | 10 | 11.8 |
| NS3-0-N | 2019 | Labrador Shelf | NS | Pelagic | Seawater | > 3 | 4 | 5.0 |
| NS3-1-N | 2019 | Labrador Shelf | NS | Pelagic | Seawater | > 3 | 20 | 7.4 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample ID** | **Year** | **Location** | **Station** | **Algae type** | **Samples** | **Size (μm)** | **Depth (m)** | **Biomass (mg)** |
| NS3-0.5-P | 2019 | Labrador Shelf | NS | Pelagic | Seawater | 0.2-3 | 10 | 2.7 |
| NS3-0-P | 2019 | Labrador Shelf | NS | Pelagic | Seawater | 0.2-3 | 4 | 6.1 |
| NS3-1-P | 2019 | Labrador Shelf | NS | Pelagic | Seawater | 0.2-3 | 20 | 5.3 |
| CF-Sm1 | 2021 | Baffin Bay | CF | Sea ice | Brash ice | > 3 | 0 | NA |
| CF-Sp1 | 2021 | Baffin Bay | CF | Sea ice | Brash ice | 0.2-3 | 0 | NA |
| CF0-Pm1 | 2021 | Baffin Bay | CF | Pelagic | Seawater | > 3 | 0 | NA |
| CF1-Pm1 | 2021 | Baffin Bay | CF | Pelagic | Seawater | > 3 | 27 | NA |
| CF0-Pp1 | 2021 | Baffin Bay | CF | Pelagic | Seawater | 0.2-3 | 0 | NA |
| CF1-Pp1 | 2021 | Baffin Bay | CF | Pelagic | Seawater | 0.2-3 | 27 | NA |
| SF-Sm1 | 2021 | Baffin Bay | SF | Sea ice | Brash ice | > 3 | 0 | NA |
| SF-Sp1 | 2021 | Baffin Bay | SF | Sea ice | Brash ice | 0.2-3 | 0 | NA |
| SF0-Pm1 | 2021 | Baffin Bay | SF | Pelagic | Seawater | > 3 | 0 | NA |
| SF1-Pm1 | 2021 | Baffin Bay | SF | Pelagic | Seawater | > 3 | 42 | NA |
| SF0-Pp1 | 2021 | Baffin Bay | SF | Pelagic | Seawater | 0.2-3 | 0 | NA |
| SF1-Pp1 | 2021 | Baffin Bay | SF | Pelagic | Seawater | 0.2-3 | 42 | NA |

Table S2 δ13C-AA values of fast ice, brash ice, and pelagic algae.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample ID** | **Samples** | **Phe** | **Thr** | **Ile** | **Leu** | **Val** | **Asx** | **Glx** | **Pro** | **Ala** | **Gly** | **Lys** |
| IC1-H-Apr | Fast ice | -26.5 | -7.3 | -14.8 | -27.7 | -21.3 | -13.6 | -17.6 | -21.3 | -16.8 | -16.8 | -13.4 |
| IC1-H-May | Fast ice | -30.1 | -9.4 | -22.3 | -29.0 | -26.5 | -18.4 | -20.2 | -24.2 | -19.0 | -19.3 | -17.2 |
| IC2-L-Apr | Fast ice | -31.2 | -9.1 | -20.9 | -30.7 | -25.4 | -16.7 | -21.8 | -23.9 | -18.0 | -18.6 | -16.7 |
| IC2-L-May | Fast ice | -30.6 | -8.7 | -14.7 | -29.1 | -25.5 | -16.7 | -20.3 | -23.9 | -18.5 | -18.2 | -16.3 |
| IC4-L-Apr | Fast ice | -32.7 | -10.4 | -18.6 | -31.5 | -25.6 | -17.0 | -19.9 | -24.5 | -20.8 | -18.1 | -18.0 |
| IC4-L-May | Fast ice | -31.3 | -8.3 | -20.0 | -28.7 | -25.3 | -18.1 | -19.4 | -22.7 | -19.1 | -15.5 | -18.3 |
| ICEn1a | Brash ice | -33.2 | -13.5 | -25.1 | -31.4 | -28.4 | -14.0 | -23.4 | -23.3 | -21.5 | -17.3 | -22.3 |
| ICEn1b | Brash ice | -28.5 | -9.8 | -20.5 | -31.1 | -28.8 | -15.8 | -21.9 | -23.4 | -22.1 | -18.6 | -19.5 |
| ICEn2a | Brash ice | -28.7 | -12.8 | -22.0 | -30.7 | -28.9 | -15.9 | -20.8 | -23.4 | -21.7 | -20.9 | -18.6 |
| ICEn2b | Brash ice | -28.4 | -14.0 | -20.0 | -31.6 | -29.5 | -16.1 | -22.2 | -23.8 | -23.0 | -19.8 | -18.7 |
| ICEn3a | Brash ice | -30.0 | -11.8 | -26.1 | -30.3 | -29.6 | -17.0 | -21.1 | -23.8 | -19.7 | -19.0 | -19.9 |
| ICEn3b | Brash ice | -27.2 | -12.0 | -18.9 | -29.5 | -28.1 | -15.0 | -19.7 | -22.2 | -19.6 | -17.1 | -17.2 |
| ICEp1 | Brash ice | -28.8 | -10.3 | -21.6 | -31.0 | -32.0 | -17.9 | -22.6 | -24.7 | -21.7 | -19.6 | -18.7 |
| ICEp2 | Brash ice | -31.5 | -12.9 | -28.2 | -33.3 | -33.1 | -20.8 | -25.0 | -28.1 | -21.9 | -21.8 | -19.6 |
| ICEp3 | Brash ice | -29.3 | NA | -24.4 | -30.6 | -29.7 | -17.2 | -24.0 | -24.8 | -19.3 | -16.1 | -19.1 |
| 1-15-0-N | Seawater | -30.8 | -16.5 | -26.1 | -33.0 | -32.0 | -19.5 | -22.5 | -24.7 | -22.2 | -16.0 | -19.4 |
| 1-15-1-N | Seawater | -30.1 | -16.6 | -24.0 | -32.6 | -31.6 | -19.4 | -22.0 | -24.5 | -22.1 | -13.4 | -20.6 |
| 1-15-0.5-P | Seawater | -28.7 | -15.5 | -19.0 | -30.2 | -29.6 | -19.7 | -20.3 | -23.1 | -22.3 | -11.4 | -18.2 |
| 1-15-1-P | Seawater | -28.4 | -19.5 | -27.6 | -31.5 | -29.6 | -22.2 | -22.8 | -25.6 | -23.6 | -12.4 | -21.6 |
| NS3-0.5-N | Seawater | -27.0 | -13.6 | -20.5 | -27.7 | -27.8 | -16.2 | -19.8 | -24.4 | -22.0 | -11.3 | -16.6 |
| NS3-0-N | Seawater | -28.3 | -15.3 | -21.4 | -27.4 | -27.6 | -17.6 | -19.8 | -23.4 | -22.3 | NA | -18.9 |
| NS3-1-N | Seawater | -28.0 | -14.2 | -22.2 | -27.3 | -28.1 | -16.2 | -19.7 | -23.7 | -20.6 | -12.2 | -16.5 |
| NS3-0.5-P | Seawater | -28.2 | -16.8 | -23.2 | -27.4 | -27.9 | -18.3 | -19.4 | -23.7 | -21.0 | -13.0 | -16.1 |
| NS3-0-P | Seawater | -27.5 | -16.9 | -25.4 | -28.3 | -29.2 | -19.4 | -18.9 | -23.5 | -20.4 | -11.8 | -17.7 |
| NS3-1-P | Seawater | -29.2 | -16.9 | -24.6 | -28.1 | -31.0 | -18.7 | -20.6 | -24.4 | -21.9 | -13.4 | -17.6 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample ID** | **Samples** | **Phe** | **Thr** | **Ile** | **Leu** | **Val** | **Asx** | **Glx** | **Pro** | **Ala** | **Gly** | **Lys** |
| CF-Sm1 | Brash ice | -25.6 | -9.6 | -19.1 | -24.8 | -25.7 | -15.4 | -9.2 | -18.9 | -20.9 | -14.2 | -18.5 |
| CF-Sp1 | Brash ice | -24.8 | -14.3 | -19.8 | -24.6 | -28.5 | -17.1 | -10.8 | -19.4 | -23.2 | -15.3 | -16.8 |
| CF0-Pm1 | Seawater | -26.2 | -13.0 | -19.2 | -28.7 | -28.5 | -17.6 | -16.3 | -21.6 | -20.6 | -15.1 | -21.0 |
| CF1-Pm1 | Seawater | -23.2 | -7.9 | -17.1 | -26.9 | -24.9 | -11.3 | -12.0 | -18.6 | -16.8 | -15.4 | -17.6 |
| CF0-Pp1 | Seawater | -25.4 | -13.0 | -20.0 | -25.9 | -28.1 | -17.8 | -13.4 | -20.7 | -21.9 | -16.5 | -16.9 |
| CF1-Pp1 | Seawater | -25.2 | -14.2 | -17.7 | -28.0 | -27.8 | -17.4 | -14.6 | -22.2 | -18.9 | -15.2 | -19.2 |
| SF-Sm1 | Brash ice | -25.7 | -9.9 | -19.9 | -26.1 | -27.6 | -15.2 | -6.9 | -18.9 | -20.1 | -14.5 | -21.2 |
| SF-Sp1 | Brash ice | -25.2 | -7.7 | -19.8 | -22.4 | -25.5 | -15.0 | -5.8 | -18.5 | -20.4 | -12.0 | -21.3 |
| SF0-Pm1 | Seawater | -28.2 | -15.3 | -23.2 | -26.9 | -27.0 | -20.4 | -15.4 | -23.0 | -22.9 | -15.7 | -22.2 |
| SF1-Pm1 | Seawater | -26.5 | -11.3 | -15.7 | -26.8 | -24.9 | -19.2 | -13.1 | -21.1 | -21.2 | -15.4 | -21.9 |
| SF0-Pp1 | Seawater | -30.5 | -15.5 | -16.5 | -27.5 | -30.7 | -19.5 | -14.2 | -23.7 | NA | -17.6 | -24.7 |
| SF1-Pp1 | Seawater | -27.6 | -13.0 | -21.6 | -26.4 | -28.0 | -19.5 | -13.3 | -19.7 | -23.1 | -14.9 | -21.9 |

Table S3 δ15N-AA values of brash ice and pelagic algae.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample ID** | **Samples** | **Phe** | **Thr** | **Ile** | **Leu** | **Val** | **Asx** | **Glx** | **Pro** | **Ala** | **Gly** | **Lys** |
| ICEn1a | Brash ice | 7.0 | 5.4 | 5.8 | 4.4 | 12.0 | 6.2 | 11.5 | 8.3 | 6.4 | 5.4 | 6.8 |
| ICEn1b | Brash ice | 4.9 | 3.6 | 5.6 | 2.4 | 10.9 | 4.6 | 8.8 | 6.2 | 6.1 | 4.4 | 4.7 |
| ICEn2a | Brash ice | 6.5 | 5.0 | 4.8 | 3.9 | 12.5 | 6.2 | 11.0 | 7.5 | 6.8 | 5.3 | 6.6 |
| ICEn2b | Brash ice | 6.0 | 3.5 | 6.6 | 3.7 | 11.7 | 5.5 | 9.5 | 6.7 | 6.4 | 5.1 | 4.9 |
| ICEn3a | Brash ice | 8.0 | 7.4 | 6.3 | 4.7 | 13.7 | 7.1 | 11.1 | 6.3 | 7.2 | 6.2 | 7.5 |
| ICEn3b | Brash ice | 5.0 | 5.0 | 5.4 | 2.8 | 12.6 | 5.3 | 9.0 | 5.1 | 6.5 | 6.2 | 5.6 |
| ICEp1 | Brash ice | 4.6 | 4.0 | 4.4 | 5.2 | 12.8 | 5.7 | 10.0 | 6.9 | 6.2 | 5.1 | 5.0 |
| ICEp3 | Brash ice | 7.4 | NA | 4.7 | 4.5 | 13.5 | 6.8 | 11.7 | 8.1 | 7.5 | 5.6 | 7.6 |
| 1-15-0-N | Seawater | 4.7 | 2.2 | 8.3 | 3.8 | NA | 6.8 | 8.7 | 7.5 | 8.2 | 3.5 | 4.7 |
| 1-15-1-N | Seawater | 2.6 | 0.8 | NA | 5.1 | NA | 7.1 | 10.0 | 6.9 | 8.8 | 2.8 | 4.2 |
| 1-15-0.5-P | Seawater | 5.1 | 0.9 | NA | 3.8 | NA | 7.2 | 10.2 | 8.7 | 11.0 | 0.9 | 4.3 |
| 1-15-1-P | Seawater | 3.0 | -0.1 | 4.9 | 3.6 | 9.4 | 6.6 | 9.5 | 8.2 | 12.1 | 1.8 | 3.6 |
| 1-15-0-P | Seawater | 4.1 | 2.4 | 6.0 | 3.5 | 9.8 | 6.5 | 8.3 | 7.6 | 9.7 | 2.5 | 4.3 |
| NS3-0.5-N | Seawater | 6.1 | 3.0 | 7.5 | 7.1 | 10.2 | 8.9 | 12.2 | 10.1 | 10.8 | 4.3 | 7.2 |
| NS3-0-N | Seawater | 5.4 | 2.6 | 7.7 | 7.8 | 12.2 | 9.1 | 12.1 | 11.4 | 10.7 | 3.8 | 7.6 |
| NS3-1-N | Seawater | 5.2 | 3.2 | 3.7 | 3.9 | 11.3 | 7.5 | 10.2 | 7.3 | 8.3 | 3.9 | 6.2 |
| NS3-0.5-P | Seawater | 5.5 | 3.0 | 6.0 | 5.8 | 10.0 | 8.0 | 11.3 | 10.0 | 11.4 | 0.2 | 6.4 |
| NS3-0-P | Seawater | 4.3 | NA | 4.3 | 3.9 | 10.2 | 7.1 | 9.5 | 10.9 | 10.0 | 1.2 | 5.8 |
| NS3-1-P | Seawater | 4.1 | 1.5 | 4.9 | 5.3 | 9.7 | 7.0 | 10.0 | 9.2 | 9.3 | 1.1 | 5.4 |
| CF-Sm1 | Brash ice | 6.9 | 0.9 | 7.5 | 7.1 | 12.7 | 8.5 | 10.2 | 13.5 | 12.7 | 6.9 | 4.7 |
| CF-Sp1 | Brash ice | 7.3 | 3.8 | 7.1 | 7.0 | 13.4 | 9.6 | 11.9 | 13.5 | 15.1 | 4.3 | 5.8 |
| CF0-Pm1 | Seawater | 7.7 | NA | NA | 6.9 | NA | 11.2 | 12.6 | 11.3 | NA | 6.7 | 7.0 |
| CF1-Pm1 | Seawater | 4.8 | 5.9 | 4.6 | 3.5 | 12.1 | 8.5 | 11.1 | 8.2 | 10.5 | 4.8 | 5.9 |
| CF0-Pp1 | Seawater | 5.6 | 5.9 | 4.2 | 5.9 | 11.4 | 9.9 | 12.4 | 12.6 | 12.7 | 4.1 | NA |
| CF1-Pp1 | Seawater | 6.0 | NA | NA | 6.7 | NA | 11.3 | 15.8 | 12.6 | NA | 6.6 | 7.4 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample ID** | **Samples** | **Phe** | **Thr** | **Ile** | **Leu** | **Val** | **Asx** | **Glx** | **Pro** | **Ala** | **Gly** | **Lys** |
| SF-Sm1 | Brash ice | 4.0 | 2.4 | 4.4 | 4.5 | 10.7 | 5.7 | 7.7 | 10.0 | 8.9 | 3.2 | 3.0 |
| SF-Sp1 | Brash ice | 4.6 | 3.5 | 3.3 | 3.8 | 10.6 | 6.1 | 8.0 | 10.1 | 10.9 | 1.9 | 2.3 |
| SF0-Pm1 | Seawater | 4.8 | NA | NA | 5.0 | NA | 8.0 | 9.8 | 10.1 | NA | 3.6 | 5.2 |
| SF1-Pm1 | Seawater | 6.1 | 3.7 | 7.0 | 7.4 | 12.5 | 10.4 | 13.5 | 11.3 | 13.4 | 4.9 | 6.4 |
| SF0-Pp1 | Seawater | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| SF1-Pp1 | Seawater | 5.4 | NA | NA | 7.1 | NA | 9.4 | 13.3 | 11.5 | NA | NA | 5.8 |



**Figure S1.** The AA molar composition of pelagic algae (P) and sea ice algae from the fast ice (F) and brash ice (B). Error bars represent ± 1 s.d. of averages of samples (n = 5-9).

Table S4 Principal component analysis output for Fig. 4b.

|  |
| --- |
| **Importance of components** |
|  | PC1 | PC2 | PC3 | PC4 | PC5 |
| Eigenvalue | 2.43 | 1.23 | 0.86 | 0.47 | 0.00 |
| Cumulative portion | 0.49 | 0.73 | 0.91 | 1.00 | 1.00 |
|  |  |  |  |  |  |
| **Vector scores** |
|  | PC1 | PC2 | PC3 | PC4 | PC5 |
| Phe | -0.56 | 0.04 | -0.20 | -0.66 | 0.46 |
| Leu | -0.54 | -0.18 | 0.16 | 0.69 | 0.42 |
| Thr | 0.48 | -0.24 | -0.64 | 0.14 | 0.53 |
| Ile | 0.28 | 0.77 | 0.32 | 0.05 | 0.48 |
| Val | 0.30 | -0.57 | 0.65 | -0.26 | 0.33 |
|  |  |  |  |  |  |
| **Sample scores** |  |  |  |  |  |
| Sample ID | PC1 | PC2 | PC3 | PC4 | Group |
| ICEp1a | 0.42 | 1.19 | -2.55 | 0.09 | B |
| ICEp2a | 0.12 | -1.12 | -2.25 | -0.15 | B |
| ICEn1a | 1.36 | -1.75 | 0.52 | 0.40 | B |
| ICEn2a | 0.36 | -0.04 | -0.37 | -0.55 | B |
| ICEn3a | 0.11 | -1.70 | -1.18 | 0.08 | B |
| ICEn1b | 1.35 | 0.45 | -1.29 | -0.54 | B |
| ICEn3b | 0.38 | 1.00 | -0.30 | -0.57 | B |
| ICEn2b | 0.43 | 1.24 | -0.11 | -0.95 | B |
| CF-Sp1 | -2.56 | 0.80 | 0.03 | 0.52 | B |
| CF-Sm1 | -0.48 | -0.29 | -0.33 | 0.59 | B |
| SF-Sp1 | -0.96 | -0.89 | -1.00 | 1.48 | B |
| SF-Sm1 | -0.66 | 0.15 | -1.09 | 0.36 | B |
| IC1-H-May | 1.50 | -1.43 | -0.35 | 0.41 | F |
| IC4-L-May | 2.60 | -1.06 | 0.18 | 0.87 | F |
| IC2-L-May | 3.13 | 1.38 | 0.61 | 0.69 | F |
| IC1-H-Apr | 2.80 | -0.12 | 1.17 | -0.80 | F |
| IC2-L-Apr | 2.82 | -1.24 | 0.23 | -0.03 | F |
| IC4-L-Apr | 3.51 | -0.13 | 1.10 | 0.14 | F |
| NS3L-0-N | -0.94 | -0.21 | 1.12 | 0.25 | P |
| NS3L-0.5-N | -0.76 | 0.22 | 0.29 | -0.09 | P |
| NS3L-1-N | -1.06 | -0.45 | 0.39 | 0.35 | P |
| NS3L-0-P | -2.19 | -1.15 | 0.51 | -0.37 | P |
| NS3L-0.5-P | -1.64 | -0.76 | 1.35 | 0.12 | P |
| NS3L-1-P | -2.07 | -0.24 | 0.13 | 0.66 | P |
| 1-15-1-N | -0.37 | 0.43 | -0.14 | -0.73 | P |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Sample scores** |  |  |  |  |  |
| Sample ID | PC1 | PC2 | PC3 | PC4 | Group |
| 1-15-0\_5-P | -0.10 | 1.68 | 0.58 | -0.32 | P |
| 1-15-0-N | -0.45 | -0.38 | -0.40 | -0.67 | P |
| 1-15-1-P | -1.98 | -1.64 | 1.14 | -1.55 | P |
| CF1-Pp1 | -0.91 | 1.58 | 0.45 | -0.75 | P |
| CF1-Pm1 | 0.35 | 0.42 | -0.90 | -1.04 | P |
| CF0-Pp1 | -1.60 | 0.52 | -0.24 | 0.20 | P |
| CF0-Pm1 | -0.52 | 1.13 | -0.26 | -0.59 | P |
| SF1-Pp1 | -1.08 | -0.34 | -0.02 | 0.68 | P |
| SF1-Pm1 | 0.67 | 1.04 | 1.06 | -0.09 | P |
| SF0-Pp1 | -0.34 | 2.93 | 0.76 | 1.66 | P |
| SF0-Pm1 | -1.25 | -1.24 | 1.16 | 0.24 | P |

Table S5 Linear discriminant analysis output for Fig. 5.

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| --- |
| **Coefficients of linear discriminants** |
|  | LD1 | LD2 |  |  |
| Phe | -2.22 | 58.2 |  |  |
| Thr | -3.11 | 58.6 |  |  |
| Ile | -2.84 | 57.9 |  |  |
| Leu | -2.69 | 58.2 |  |  |
| Val | -3.19 | 57.5 |  |  |
|  |  |  |  |  |
| **Proportion of trace** |
|  | LD1 | LD2 |  |  |
|  | 0.80 | 0.20 |  |  |
|  |  |  |  |  |
| **Posterior probabilities with leave-one-out cross validation of the classifier samples** |
| Sample ID | Actual | Predicted (% probability) |
|  |  | Brash ice algae (B) | Fast ice algae (F) | Pelagic algae (P) |
| ICEp1a | B | **99.8** | 0.0 | 0.2 |
| ICEp2a | B | **99.9** | 0.0 | 0.1 |
| ICEn1a | B | 0.0 | **100.0** | 0.0 |
| ICEn2a | B | **61.7** | 0.1 | 38.2 |
| ICEn3a | B | **94.9** | 0.2 | 4.8 |
| ICEn1b | B | **91.0** | 1.5 | 7.4 |
| ICEn2b | B | 21.5 | 0.0 | **78.5** |
| ICEn3b | B | 32.5 | 0.0 | **67.5** |
| CF-Sp1 | B | 0.0 | 0.0 | **100.0** |
| CF-Sm1 | B | **81.5** | 0.0 | 18.5 |
| SF-Sp1 | B | **82.4** | 0.0 | 17.6 |
| SF-Sm1 | B | **84.4** | 0.0 | 15.6 |
| IC1-H-May | F | 35.8 | **62.9** | 1.3 |
| IC4-L-May | F | 0.0 | **100.0** | 0.0 |
| IC2-L-May | F | 0.1 | **99.9** | 0.0 |
| IC1-H-Apr | F | 0.1 | **99.8** | 0.1 |
| IC2-L-Apr | F | 0.1 | **99.9** | 0.0 |
| IC4-L-Apr | F | 0.0 | **100.0** | 0.0 |
| NS3L-0-N | P | 2.5 | 0.0 | **97.5** |
| NS3L-0.5-N | P | 10.8 | 0.0 | **89.2** |
| NS3L-1-N | P | 15.8 | 0.0 | **84.2** |
| NS3L-0-P | P | 2.0 | 0.0 | **98.0** |
| NS3L-0.5-P | P | 0.6 | 0.0 | **99.4** |

|  |
| --- |
| **Posterior probabilities with cross validation of the classifier samples** |
| Sample ID | Actual | Predicted (% probability) |
|  |  | Brash ice algae (B) | Fast ice algae (F) | Pelagic algae (P) |
| NS3L-1-P | P | 10.1 | 0.0 | **89.9** |
| 1-15-1-N | P | **57.5** | 0.0 | 42.5 |
| 1-15-0\_5-P | P | 1.2 | 0.0 | **98.8** |
| 1-15-0-N | P | 28.7 | 0.0 | **71.3** |
| 1-15-1-P | P | 0.4 | 0.0 | **99.6** |
| CF1-Pp1 | P | 0.2 | 0.0 | **99.8** |
| CF1-Pm1 | P | **89.6** | 0.0 | 10.4 |
| CF0-Pp1 | P | 5.5 | 0.0 | **94.5** |
| CF0-Pm1 | P | 17.9 | 0.0 | **82.1** |
| SF1-Pp1 | P | 43.2 | 0.0 | **56.8** |
| SF1-Pm1 | P | 9.6 | 1.1 | **89.3** |
| SF0-Pp1 | P | **67.1** | 0.1 | 32.8 |
| SF0-Pm1 | P | 1.1 | 0.0 | **98.9** |

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