Supporting Information for:

Molecular insights on dissolved organic matter transformation by supraglacial microbial communities

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Contents - Additional details on Materials and Methods, 1 Table and 3 figures

FTICR-MS analysis

Samples were analysed using a Bruker Daltonics 12 T Apex Qe FTICR-MS instrument, operated in both negative and positive electrospray ionisation modes, using parameters consistent with those described previously (Antony *et al.*, 2014). Prior to analysis, DOM extracts and respective field blanks were reconstituted in 50% methanol with either 0.1% NH_4OH or 0.1% HCOOH for negative and positive ion modes, respectively. The instrument was externally calibrated with a polyethylene glycol standard and internally calibrated with fatty acids and other naturally present homologous series detected within the sample (Sleighter *et al.*, 2008). All peaks found in each mode's field blank were removed from the DOM peak list. The blank-corrected master peak lists for each sample were assigned unique molecular formulas using an in-house developed MatLab code. Formula matches were generated using the criteria $^{12}C_{5\text{-}80}$, $^{1}H_{5\text{-}200}$, $^{16}O_{1\text{-}30}$, $^{14}N_{0\text{-}5}$, $^{32}S_{0\text{-}2}$, $^{34}P_{0\text{-}2}$ for negative ESI and $^{12}C_{5\text{-}80}$, $^{1}H_{5\text{-}200}$, $^{16}O_{1\text{-}30}$, $^{14}N_{0\text{-}5}$, $^{32}S_{0\text{-}2}$, $^{23}Na_{0\text{-}1}$ for positive ESI, where the subscripts indicate the range of atoms allowed in a single formula. Only m/z values with a signal to noise (S/N) above 3 were utilised. For all samples, 68-89% of all peaks were assigned a unique molecular formula. The majority (>83%) of the assigned formulas were within 0.5 ppm mass accuracy, and all formulas were within 1.0 ppm mass accuracy.

Table S1. Molecular information for DOM in the initial sample and in the 55-day biocide amended and un-amended treatment*.

Property	Initial sample	55-Day	
		Microbe + biocide	Microbe - only
Total identified formulas	2338	1759	494
C	25	22	24
H	8	6	7
O	38	36	35
P	0.03	0.03	0.06
S	0.25	0.20	0.32
N	0.29	0.62	0.44
DBE	7	5	8
DBE-O	-0.82	-0.85	1.36
AI_{mod}	0.13	0.12	0.19

* Parameters are the number of assigned molecular formulas, number-average atomic numbers per formula, double bond equivalents (DBE), DBE minus the number of oxygen atoms (DBE-O), and modified aromaticity index (AI_{mod}).

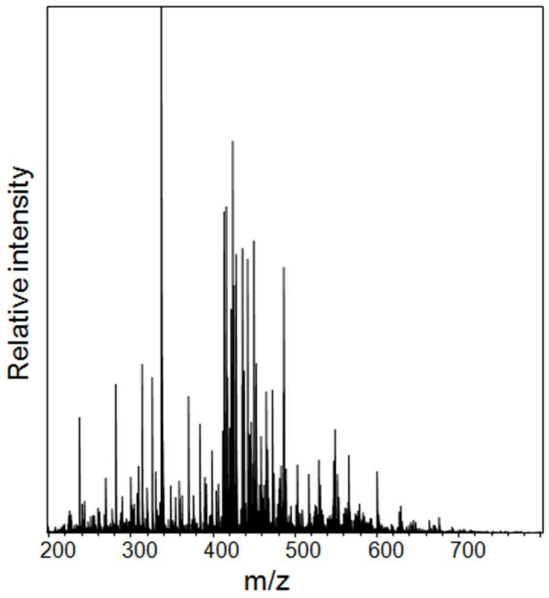

Figure S1. Ultrahigh resolution electrospray ionization Fourier transform ion cyclotron resonance mass spectrum of snowpack DOM.

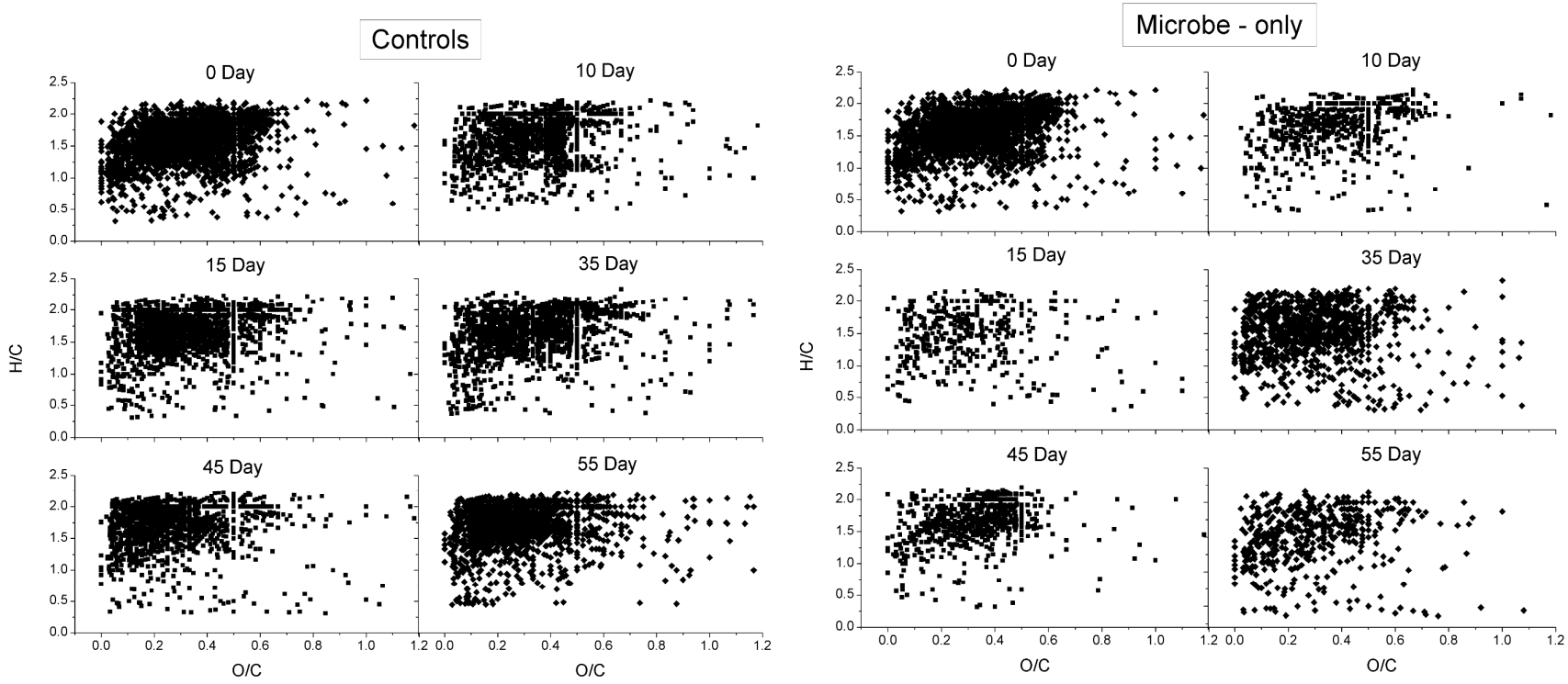

Figure S2. van Krevelen diagrams showing all identified DOM formulas at the different time points in the poisoned control and microbe-only treatments.

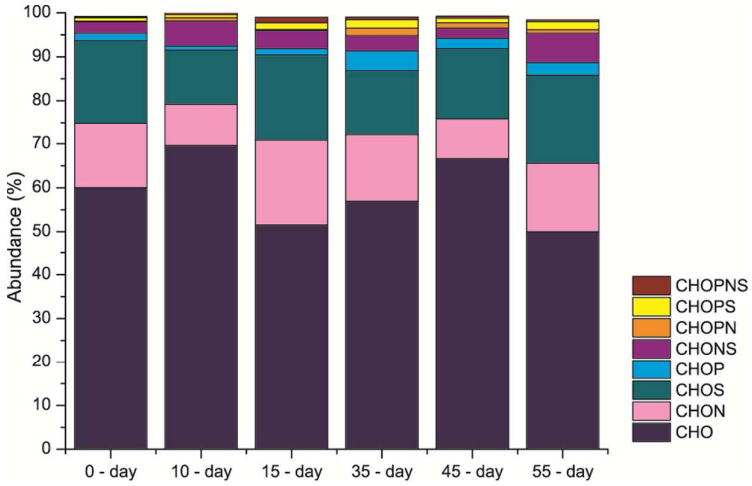

Figure S3. Percentages of each type of molecular formula present in the snowpack DOM prior to and after microbial processing.

Supplemental Material Reference:

Antony, R.; Grannas, A. M.; Willoughby, A. S.; Sleighter, R. L.; Thamban, M.; Hatcher, P. G. Origin and sources of dissolved organic matter in snow on the East Antarctic ice sheet. *Environ. Sci. Technol*. **2014**, 48, 6151–6159.

Sleighter, R. L., McKee, G. A., Liu, Z. & Hatcher, P. G. Naturally present fatty acids as internal calibrants for Fourier transform mass spectra of dissolved organic matter. *Limnol. Oceanogr.−Methods*, **6**, 246−253 (2008).