

Supplementary material for

Molecular composition of soil dissolved organic matter in recently-burned and long-unburned boreal forests

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Text S1. Chemical analysis for molecular composition of dissolved organic matter

The molecular composition of dissolved organic matter (DOM) was analysed using electrospray ionization (ESI) coupled to ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). Filtered samples were solid-phase extracted using the sorbent of styrene divinyl benzene polymer (Sep-Pak PS2 Plus Short Cartridge, Waters Inc.) according to the procedure recommended by Dittmar *et al.* (2008) to remove inorganic salts. The SPE samples were diluted with deionized water and methanol to yield a final sample composition of 50/50 (v/v) of water to methanol, and then were injected into the FT-ICR mass spectrometer (solariX 9.4T, Bruker Daltonics Inc., MA, USA) using a syringe pump (infusion rate: 100 $\mu\text{l h}^{-1}$). All samples were analysed in the negative ion mode. Ions were accumulated in a hexapole for 0.01 sec before they were transferred to the ICR cell, and the 100 transients collected using a 1 M Word time domain were co-added. All spectra were externally calibrated using a sodium iodine solution and internally calibrated using fatty acids. Each sample was analysed three times and the peak list of mass-to-charge ratio (m/z) shared among the three analytical replicates was extracted. Mass lists were produced using a signal-to-noise ratio (S/N) cut-off of 4. Isotope peaks were removed from the list. Additionally, we removed the m/z peaks derived from ultrapure water and the sampling system of soil water as described in the ‘Chemical and data analyses’ section of the main text. Molecular Formula Calculator (ver. 1.0; ©NHMFL, 1998) was used to assign an expected molecular formula for each m/z value with a mass accuracy ≤ 1 ppm. Only m/z values in the range of 180–500 were inserted into the molecular formula calculator. The following conditions were used for formula assignment: C = 0 – ∞ ; H = 0 – ∞ ; O = 0 – ∞ ; N = 0 – 5; S = 0 – 3; P = 0 – 3; DBE ≥ 0 (Grannas *et al.* 2006). After the formula assignment, some formulas not likely to be observed in natural water were eliminated based on rules described in Kujawinski and Behn (2006) and Wozniak *et al.* (2008).

References

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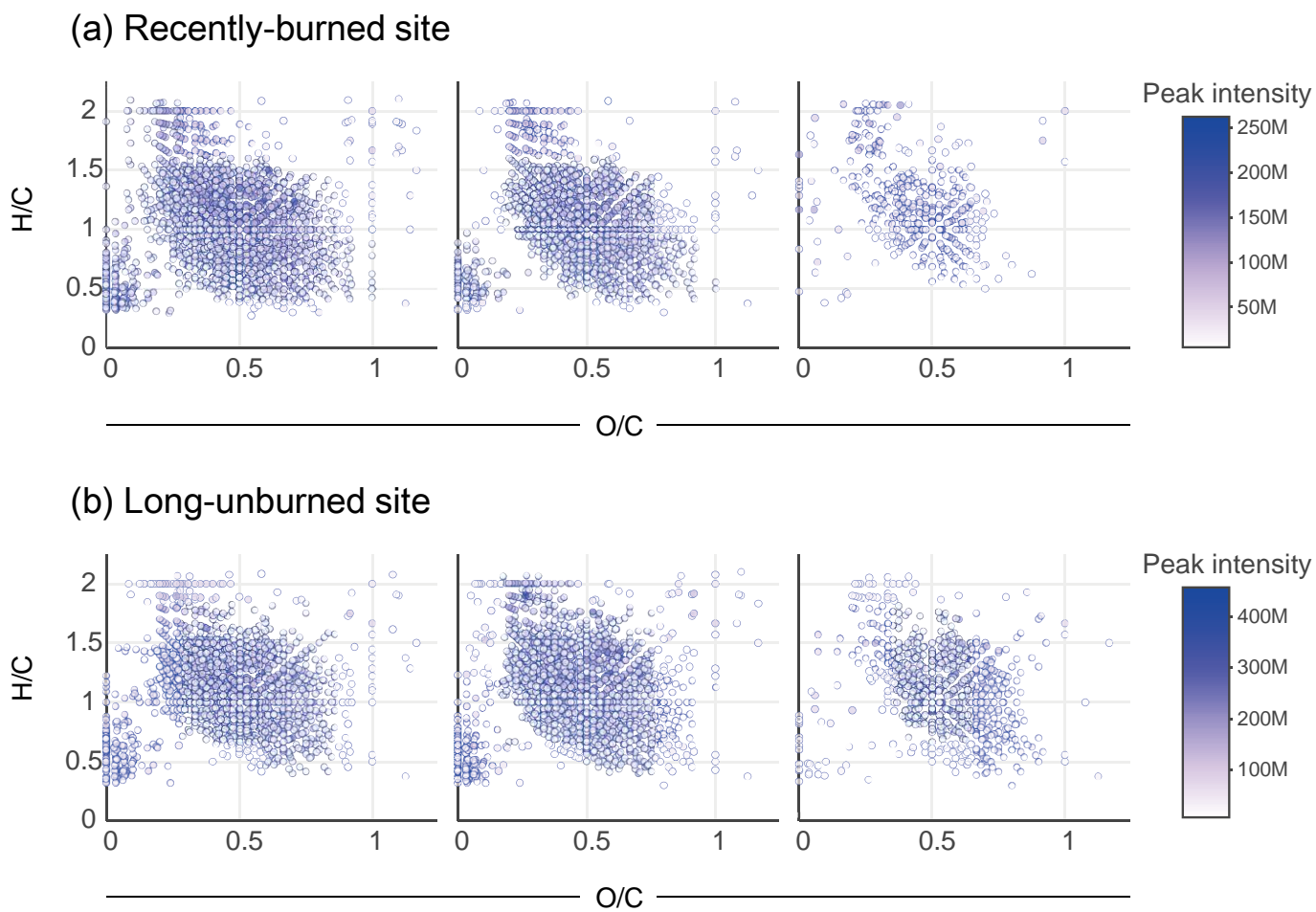


Figure S1. (a) Molecular element ratio plots (van Krevelen diagrams) of DOM samples for soil water in the recently-burned and (b) long-unburned sites.

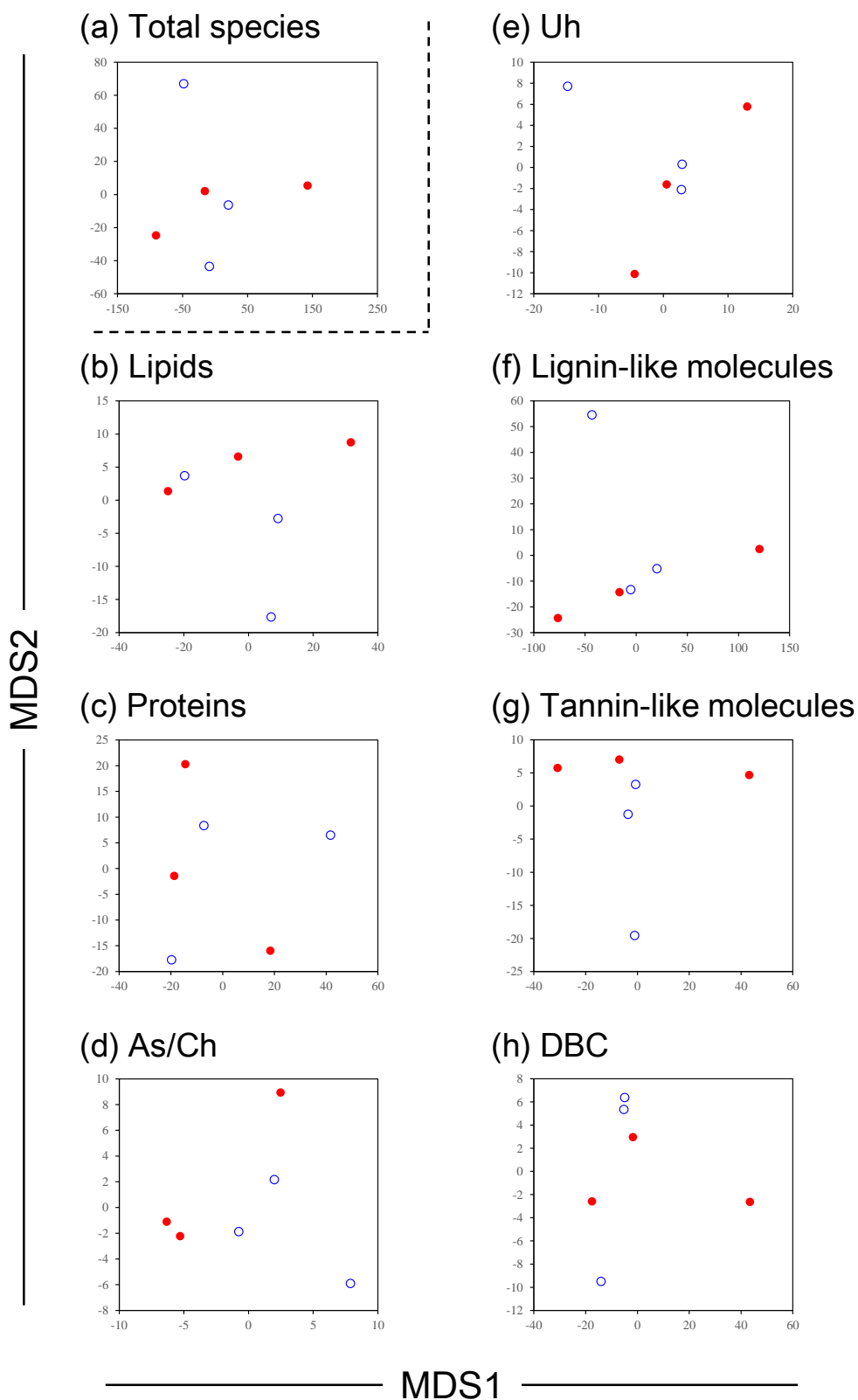


Figure S2. (a) Two-dimensional ordination of multidimensional scaling (MDS) of different sampling locations for all molecular compounds identified and (b-h) for the biomolecular classes. Closed and open circles represent soil water samples collected at the plots of recently-burned and long-unburned sites, respectively. See the Materials and methods section for the abbreviations of biomolecular classes.