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 µl 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**


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.