

S1 Text

Material and Methods: Dissolved Organic Matter analyzes. Molecular information was evaluated based on the contribution of different elements (CHO, CHON, CHOS, CHOP and CHONS formulae) and by the intensity weighted average (wa) of the Double Bond Equivalents (DBE_{wa}) and Aromaticity Index ($AI_{mod_{wa}}$) and elemental ratios H/C_{wa} and O/C_{wa} (1–3). Additionally, molecular formulae were associated with different molecular groups in order to provide an overview on the molecular composition of pore water samples (4,5). Molecular groups considered: 1) highly unsaturated compounds ($AI_{mod} < 0.5$ and $H/C < 1.5$); 2) polyphenols ($0.67 \geq AI_{mod} > 0.5$); 3) condensed aromatics or dissolved black carbon (DBC, $AI_{mod} \geq 0.67$); 4) formulae of unsaturated aliphatics ($1.5 < H/C < 2$, $O/C < 0.9$, $N=0$); 5) peptide molecular formulae ($1.5 < H/C < 2$, $O/C < 0.9$ and $N > 0$); 6) saturated fatty acids ($H/C > 2$, $O/C < 0.9$), without (saturated FA) or with heteroatoms (N, S or P) (saturated FA-CHOx); 7) formulae of sugars ($O/C > 0.9$), without (sugars) and with heteroatoms (sugars-CHOx). Furthermore, differences in composition regarding oxygen rich (O-rich) or poor (O-poor) compounds, were also evaluated.

References:

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