Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting information for

Implications of sample treatment on characterization of riverine dissolved organic matter

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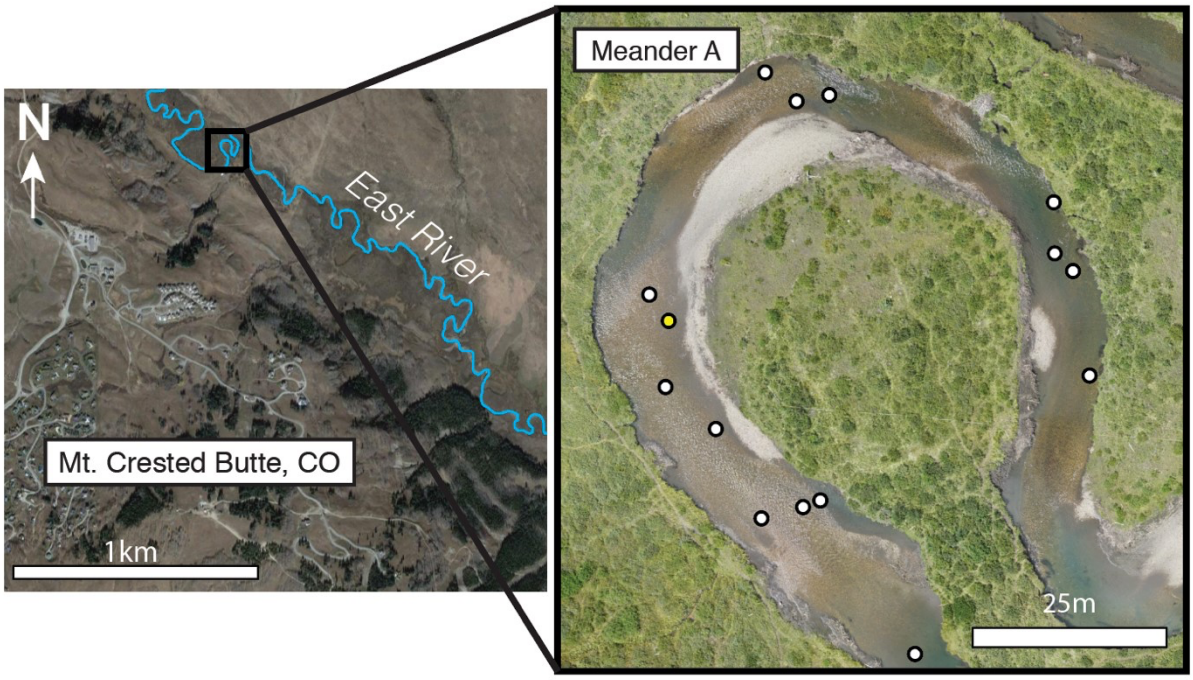

Figure S1. Sampling location of surface and pore water samples from Nelson et al. (2019) analyzed here. The sample utilized in Table 1 is highlighted.

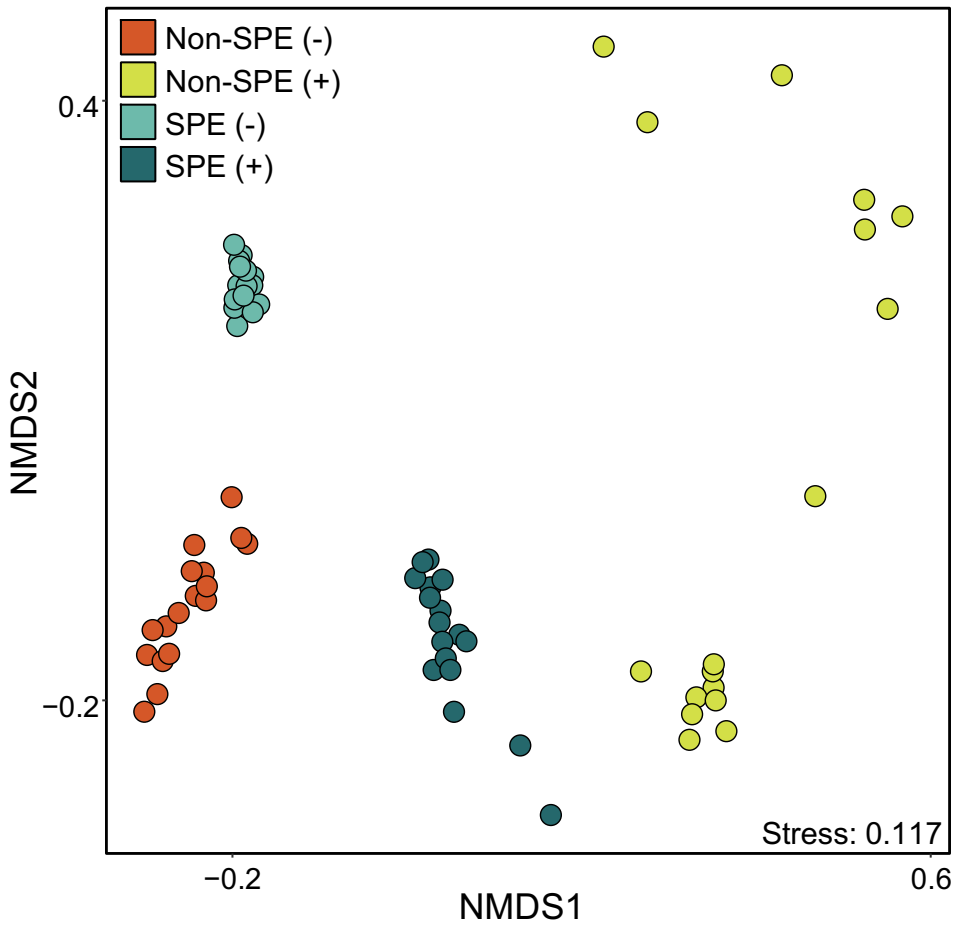

Figure S2. Non-metric multidimensional scaling ordination (NMDS) of sample set FTICR-MS data colored by method, indicating clear separation depending on chosen method.

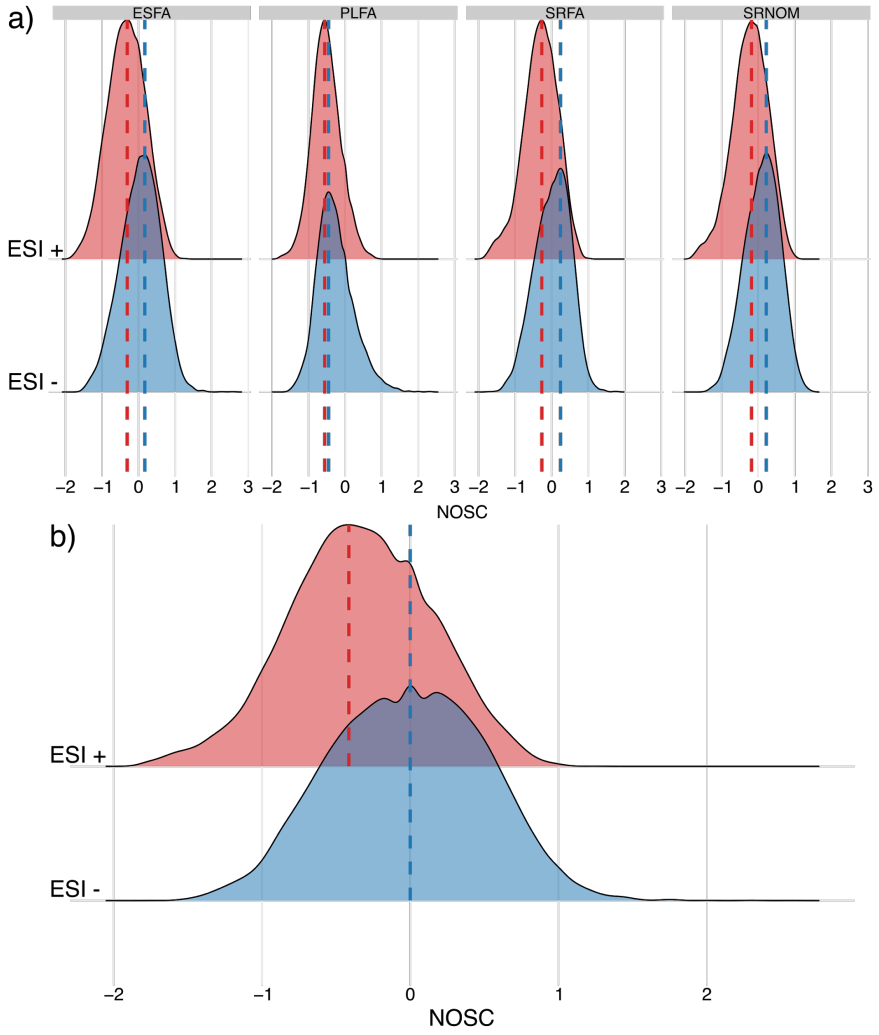

Figure S3: NOSC distributions from data obtained from Hawkes et al., 2020. a) NOSC distributions from each sample type (ESFA: Elliot Soil Fulvic Acid, PLFA: Pony Lake Fulvic Acid, SRFA: Suwannee River Fulvic Acid, SRDOM: Suwannee River Natural Organic Matter). b) NOSC distribution for combined sample types. Mann Whitney U and Kolmogorov-Smirnov Tests revealed that ESI – molecular formula had significantly higher NOSC values than ESI + molecular formula.

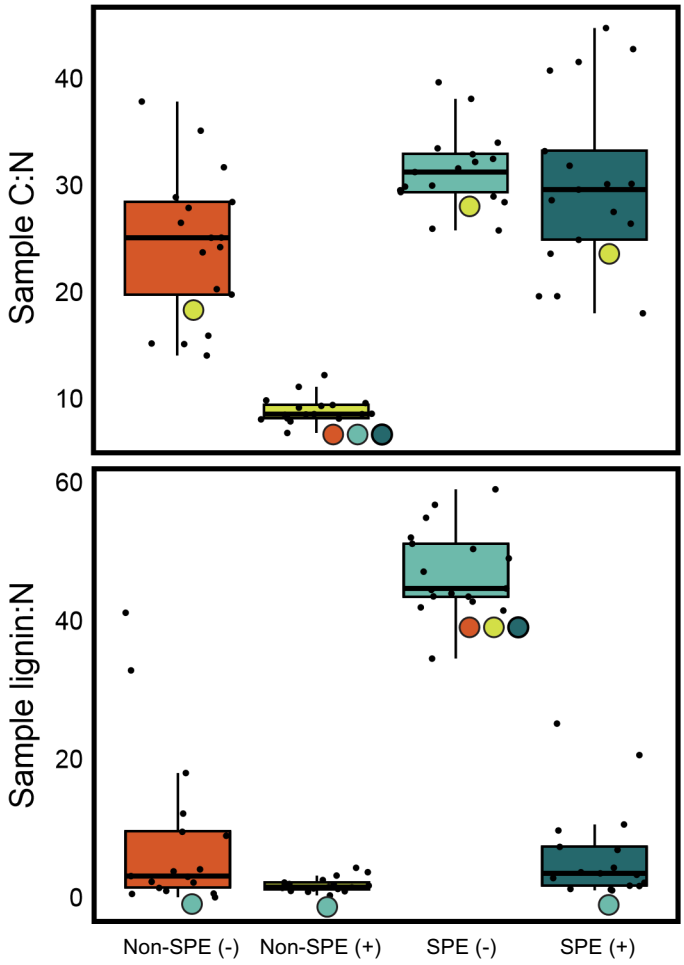

Figure S4. The distribution of sample mean C:N and lignin:N across all four FTICR-MS analysis methods. Colored circles indicate significant differences between methods.

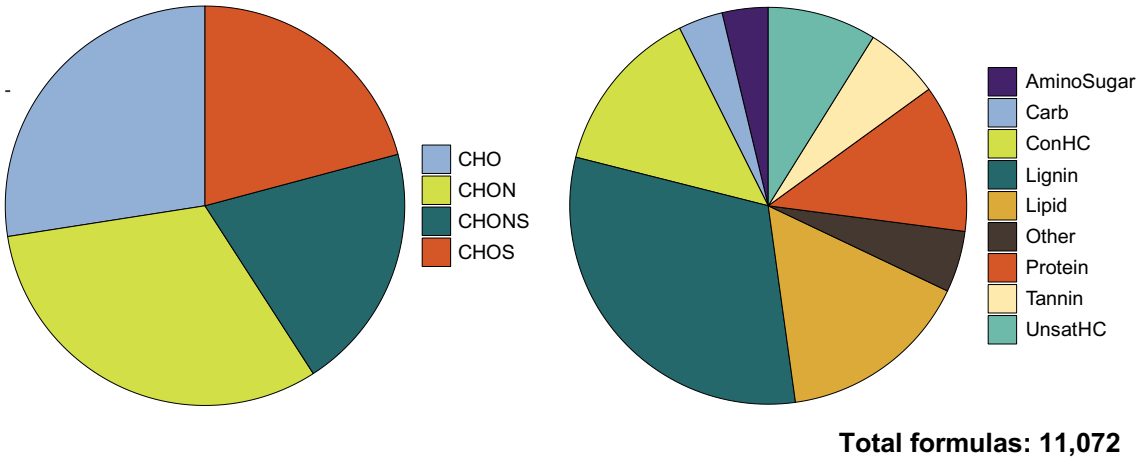

Figure S5. Distribution of composition and Van Krevelen classes of 11,072 unique formulas detected with all four methods combined.

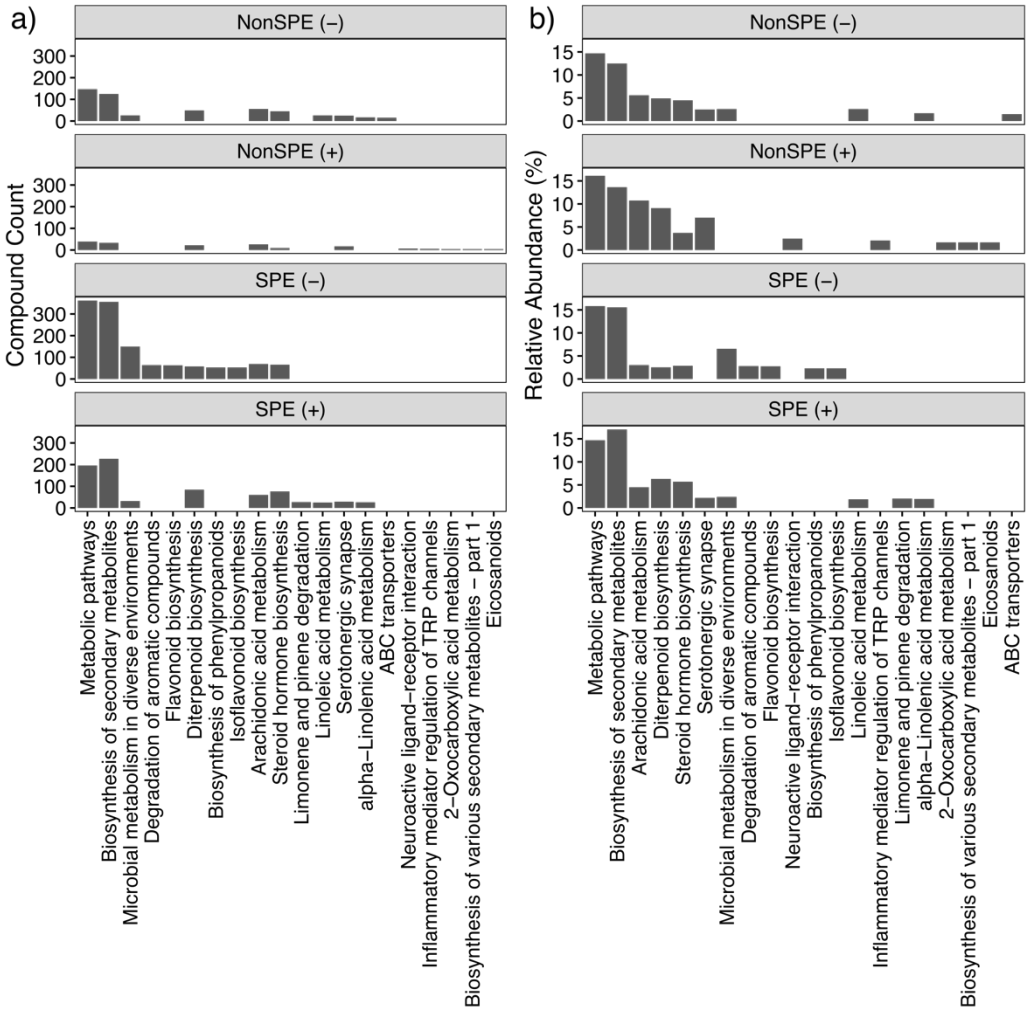

Figure S6. Comparison of metabolic pathways observed across treatment methods. a) Absolute compound counts within the 20 most represented pathways (based on actual counts). b) Relative number of compounds observed within the 20 most represented pathways (based on relative abundance).

Sample	Sampling depth (cm)	Conductivity (μS)	DOC (ppm)
A_0_cm	0	N/A	N/A
HRA	20	272.8	1.64
23A	20	289.6	2.96
B_40_cm	40	387.4	N/A
49B	20	296.7	2.48
34C	20	376.3	3.93
B_10_cm	10	268	N/A
1B	20	283.1	2.29
HOBO_10	20	278.6	1.81
HOBO_3	20	281.4	1.86
B_0_cm	0	267.8	N/A
HR4	20	285.6	1.03
36A	20	353.2	3.65
HOBO_4	20	292.7	1.06
47C	20	268.6	1.85
16A	20	269.2	1.89
50C	20	289.8	2.07

Table S1. Sample and corresponding streambed sampling depth and corresponding conductivity and DOC measurements. N/A values indicate missing measurements due to instrumental errors.

Treatment	Total Peaks	Filtered Peaks	Assigned Peaks	Unique Formulas
Non-SPE (-)	16384	13562	1257	1184
Non-SPE (+)	34156	30642	2773	2633
SPE (-)	20702	16508	6218	5916
SPE (+)	16586	13251	3629	3299

Table S2. Overview of the number of peaks from each treatment at various stages of processing. “Total Peaks” are those which were identified in the original dataset, “Filtered Peaks” are those present after using ftmsRanalysis, “Assigned Peaks” are those that were assigned some molecular formula, and “Unique Formulas” are the number of the unique molecular formulas that were assigned.

Methods	# Common Molecules
SPE +/-	881 (24.2%, 14.1%)
Non-SPE +/-	134 (4.8%, 10.6%)
Positive (SPE, Non-SPE)	511 (14.1%, 18.4%)
Negative (SPE, Non-SPE)	559 (8.9%, 44.4%)

Table S3. Number of molecules shared between indicated methods, with percentages showing the percent of formulas shared from each respective method.