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Molecular level characterisation of ion-exchange water treatment coupled to ceramic membrane filtration

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Supplementary information

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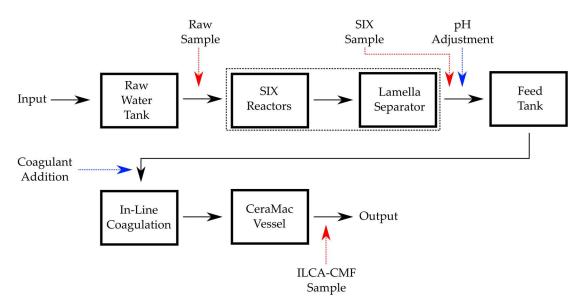


Fig. S1. Schematic setup of the pilot plant. Dashed boxed area is expanded in Fig. S9. Red arrows indicate sampling points.

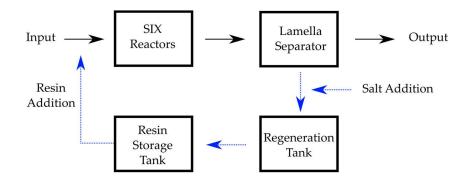


Fig. S2. A detailed diagram of the SIX treatment stage.

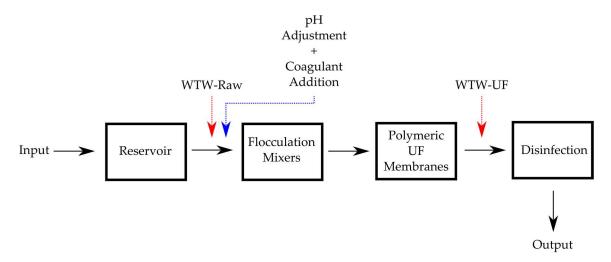


Fig. S3. A schematic diagram of the WTW. Red arrows indicate sampling points.

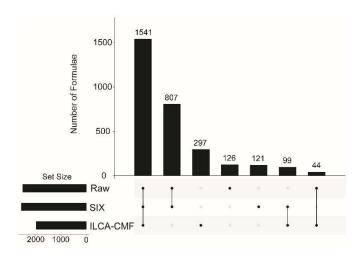


Fig. S4. Upset plot of raw, SIX and ILCA-CMF treated June pilot plant samples. Large similarities between the untreated DOM and SIX treated DOM are visible, as well as significant loss of species after the ILCA-CMF treatment.

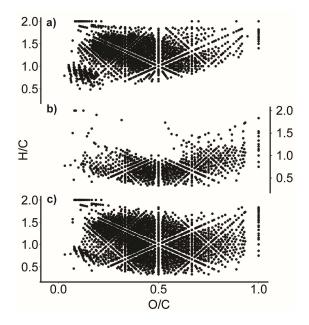


Fig. S5. Van Krevelen plots for June samples. (a) all formulae identified in the ILCA-CMF treated sample; (b) formulae lost after the ILCA-CMF treatment; (c) all formulae identified in the SIX treated sample.

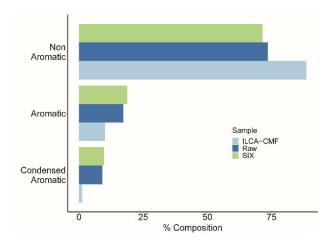


Fig. S6. AI_{mod} plot for the June pilot plant samples. There are far less condensed aromatic species present after the ILCA-CMF treatment.

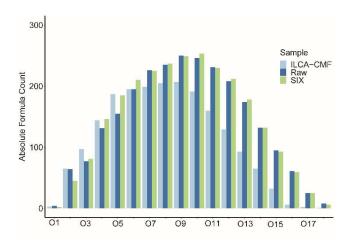


Fig. S7. Oxygen series plot for pilot plant June samples.

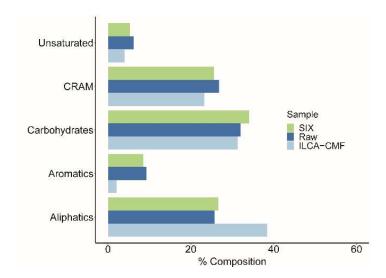


Fig. S8. Relative integrals of regions (shown in Figure 7 of the main article) of ¹H NMR spectra of the pilot plant June samples.

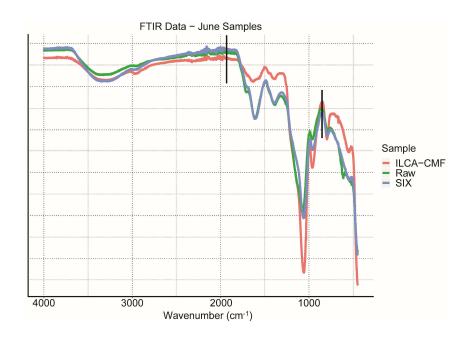


Fig. S9. ATR-FT-IR spectra of July pilot plant samples. The 800-2000 cm⁻¹ region indicated by two black lines was used for the PCA.

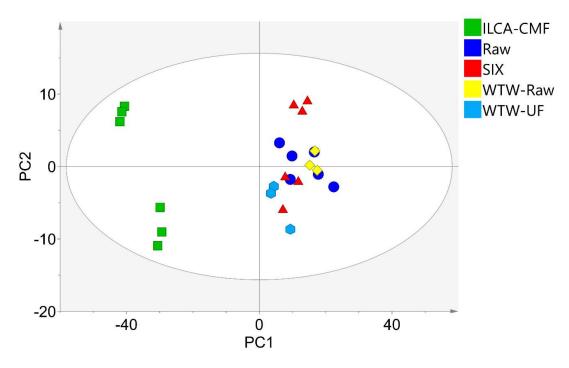


Fig. S10. PCA scores plot of the 800-2000 cm⁻¹ region of the ATR-FT-IR spectra of the July samples (identical plot to Fig.. 9a of the main article using shapes to indicate differences between sample types and not the time of collection). **Squares –** ILCA-CMF samples, **Circles –** raw samples, **Triangles –** SIX treated samples, **Diamonds –** WTW-raw samples and **hexagons –** WTW-UF samples.

Table S1. Molecular masses and formulae used to calibrate the FT-ICR-MS spectra of DOM samples.

m/z	Charge	Formula
149.060803	-1	C9H9O2
153.019332	-1	C7H5O4
259.045941	-1	C10H11O8
273.061591	-1	C11H13O8
287.077241	-1	C12H15O8
301.092891	-1	C13H17O8
315.108541	-1	C14H19O8
329.124191	-1	C15H21O8
343.139841	-1	C16H23O8
357.155491	-1	C17H25O8
371.098370	-1	C16H19O10
385.114020	-1	C17H21O10
399.129671	-1	C18H23O10
413.145321	-1	C19H25O10
427.160971	-1	C20H27O10
441.103850	-1	C19H21O12
455.119500	-1	C20H23O12
469.135150	-1	C21H25O12
483.150800	-1	C22H27O12
497.166450	-1	C23H29O12
511.182100	-1	C24H31O12
525.197750	-1	C25H33O12
539.213400	-1	C26H35O12
545.020908	-1	C23H13O16
559.036558	-1	C24H15O16
573.052208	-1	C25H17O16
587.067858	-1	C26H19O16
601.083508	-1	C27H21O16
615.099158	-1	C28H23O16
629.114808	-1	C29H25O16
643.130458	-1	C30H27O16
657.146108	-1	C31H29O16
671.161758	-1	C32H31O16
685.177409	-1	C33H33O16
699.083902	-1	C31H23O19
713.099552	-1	C32H25O19
727.115202	-1	C33H27O19
741.130852	-1	C34H29O19
755.146502	-1	C35H31O19