Supporting Information

Characterization and formation of high molecular weight disinfection byproducts in drinking water: An integrated SEC-DAD-FLD-OCD approach

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Table S1. Information of real raw water samples.

	TN (mg/L)	NH_3-N (mg/L)	DOC (mg/L)	SUVA (cm^{-1})	Cl^- (mg/L)	Br^- (mg/L)
RW1	0.25±0.01	0.15±0.01	3.58±0.05	1.58±0.10	15.68±0.12	0.05±0.01
RW2	0.63±0.01	0.13±0.01	2.21±0.05	2.53±0.15	21.83±0.12	0.03±0.01
RW3	0.63±0.01	0.23±0.01	4.26±0.05	1.92±0.10	21.27±0.12	ND

Table S2. Summary of the signs of correlations between changes of DOM fractions in the 2D Syn and aSyn maps.

Components[a]	LMWS (<0.45 kDa)	BB (0.45–1.1 kDa)	FA-II (1.1–2.0 kDa)	FA-I (2.0–2.6 kDa)	HA-II (2.6–4.0 kDa)	HA-I (4.0–7.0 kDa)
HA-I (4.0–7.0 kDa)						
HA-II (2.6–4.0 kDa)						+(+)
FA-I (2.0–2.6 kDa)					+(+)	-(+)
FA-II (1.1–2.0 kDa)				-(-)	+(+)	+(+)
BB (0.45–1.1 kDa)			+(-)	-(-)	+(-)	+(+)
LMWS (<0.45 kDa)		-(+)	-(-)	+(+)	-(+)	-(+)

[a] If the signs of the Syn and aSyn cross-peaks are identical in any given regions of the maps, the spectral change on the x axis occurs prior to the change on the y axis. The sequences are reversed if the signs of the peaks are opposite.

Table S3. Explained variance and core consistency diagnostic for different PARAFAC models.

Number of Components	Explained variance (%)	Core consistency (%)
2	86.3	92.3
3	90.1	84.3
4	92.1	74.9
5	92.7	31.4
6	93.2	5.4
7	93.4	17.6

Note: Explained variance increases with component number, whereas core consistency decreases. The four-component model was selected as the optimal solution based on a balance between high explained variance (92.1%) and acceptable core consistency (74.9%).

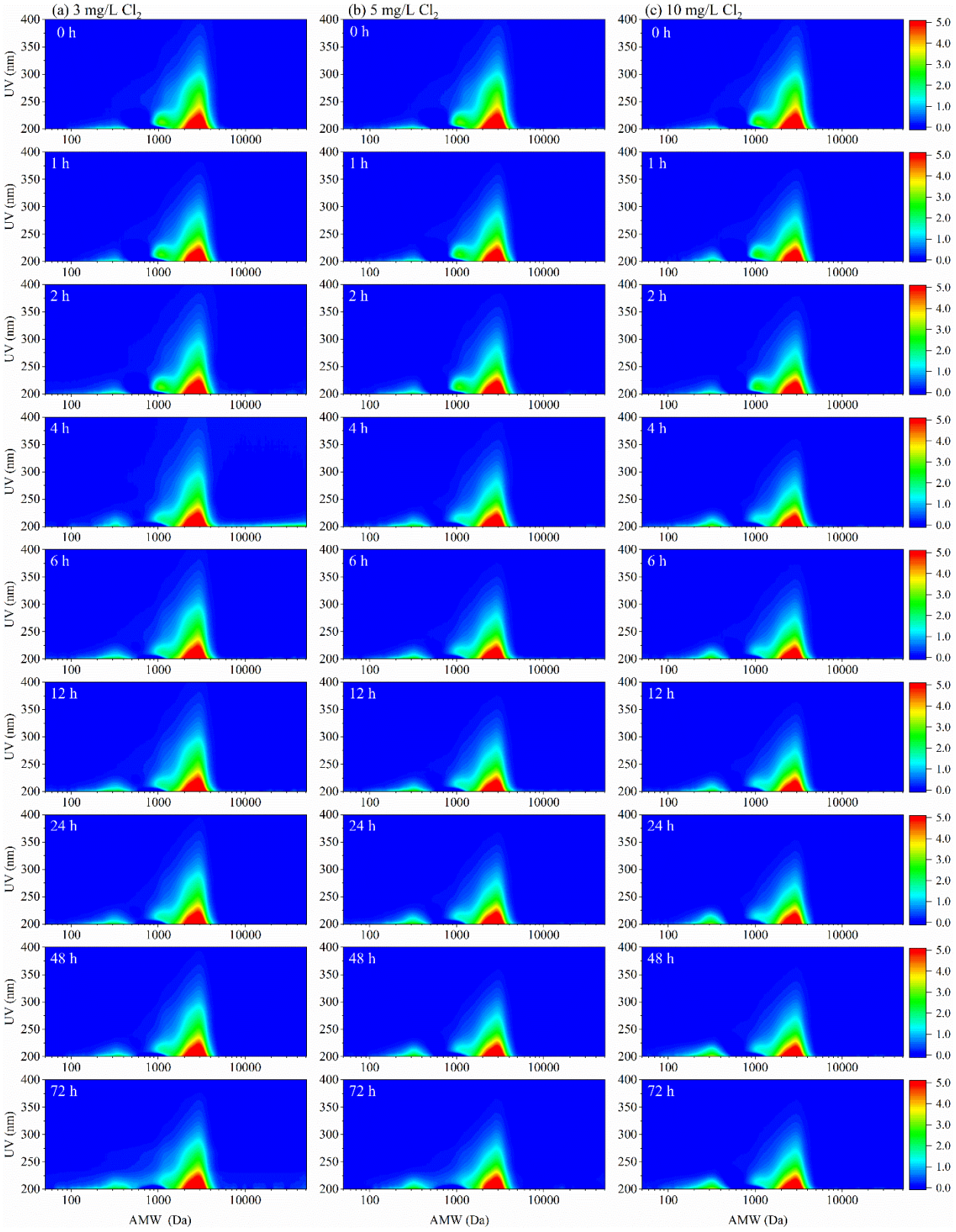

Fig. S1. SEC-DAD chromatograms of RW1 with different disinfection conditions: (a) 3 mg/L Cl_2; (b) 5 mg/L Cl_2; (c) 10 mg/L Cl_2.

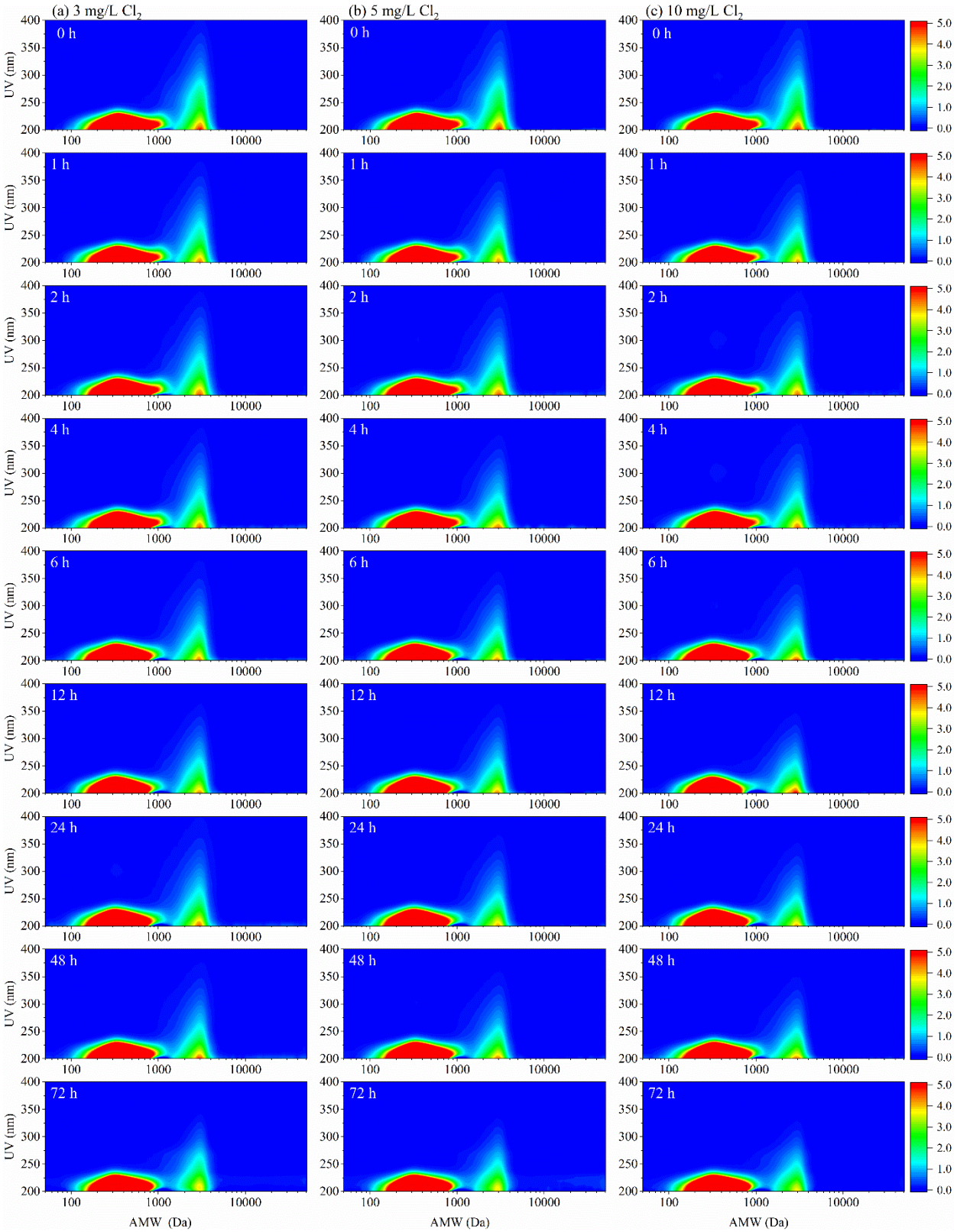

Fig. S2. SEC-DAD chromatograms of RW2 with different disinfection conditions: (a) 3 mg/L Cl_2; (b) 5 mg/L Cl_2; (c) 10 mg/L Cl_2.

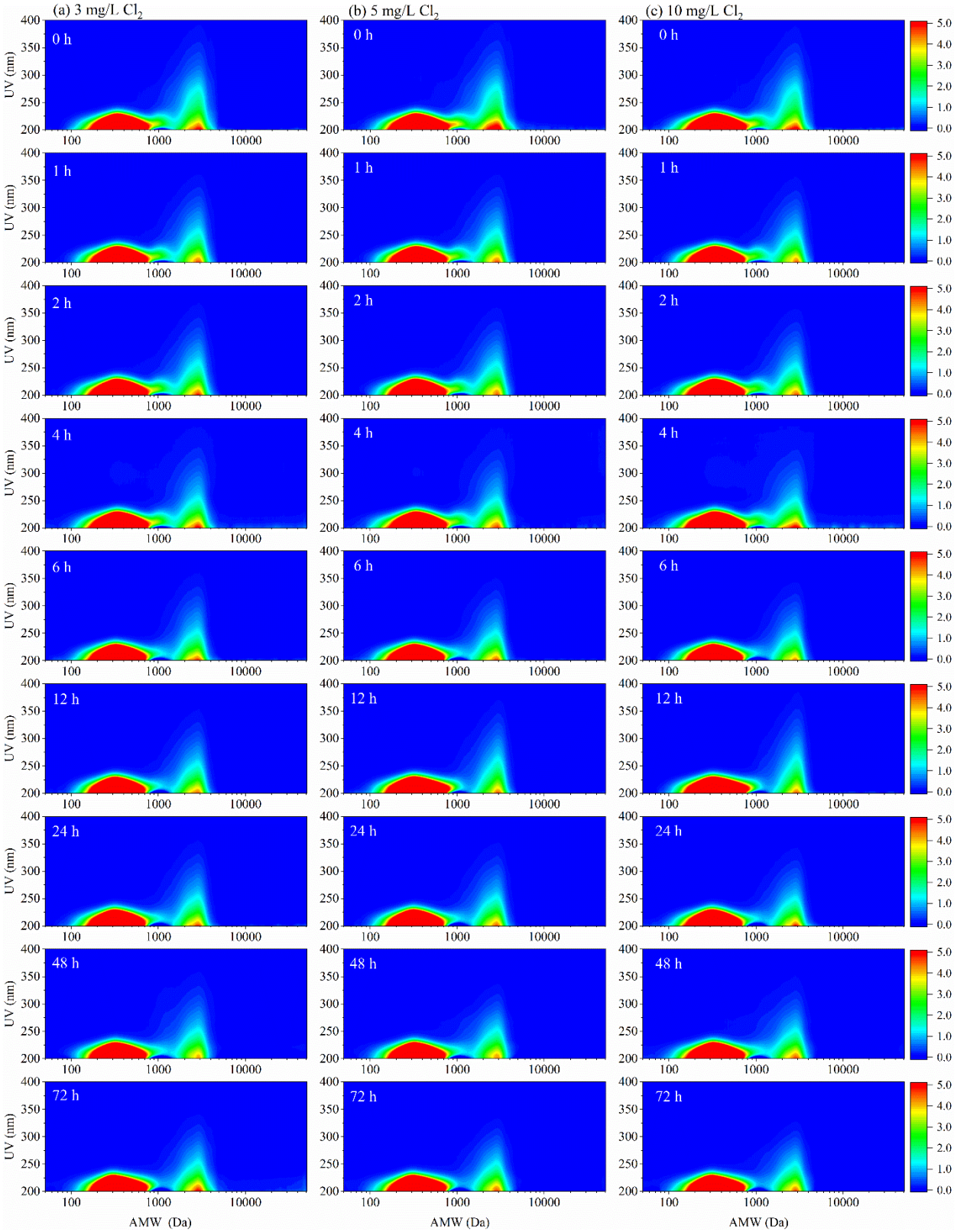

Fig. S3. SEC-DAD chromatograms of RW3 with different disinfection conditions: (a) 3 mg/L Cl_2; (b) 5 mg/L Cl_2; (c) 10 mg/L Cl_2.

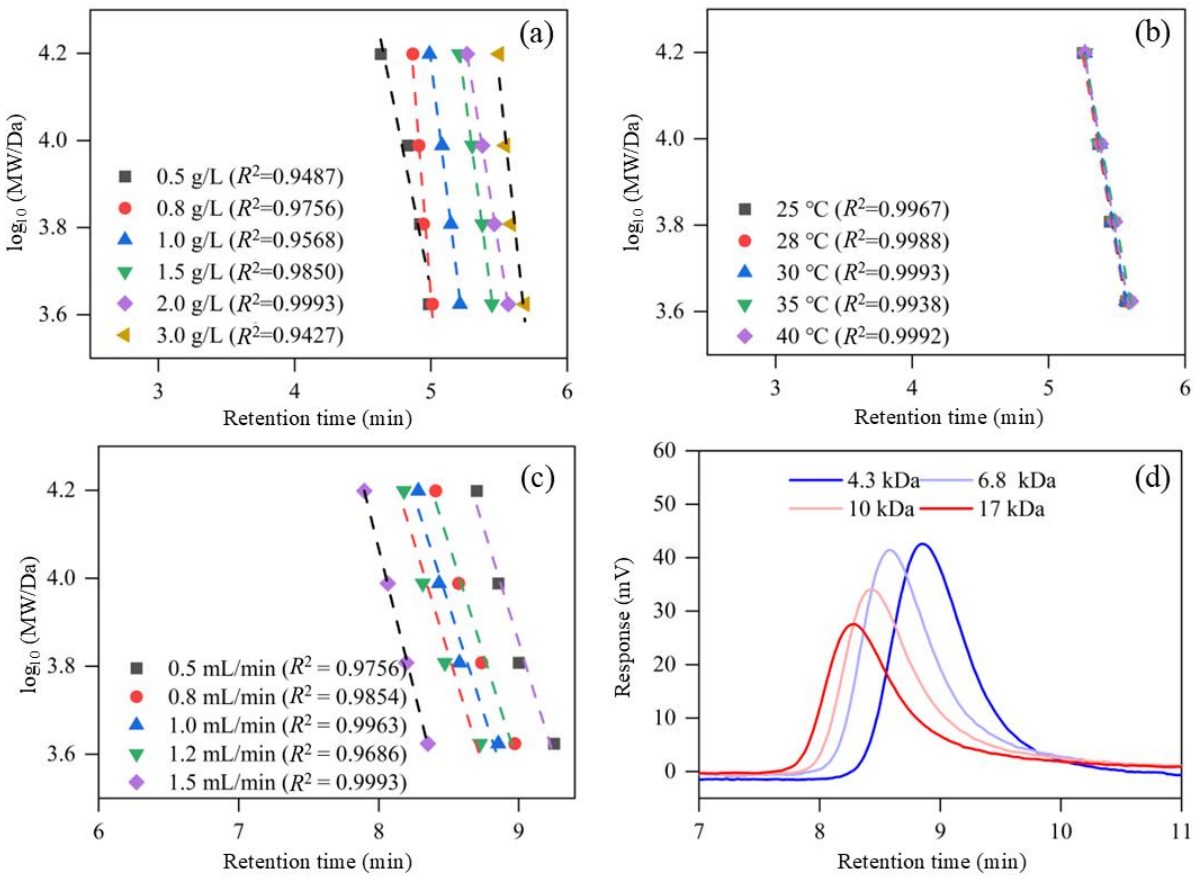

Fig. S4. SEC paramter optimization using the PL aquagel-OH 30 column: (a) effect of phosphate mobile phase (ionic strength); (b) effect of column temperature; (c) effect of flow rate; (d) optimized calibration curves obtained with PSS standards.

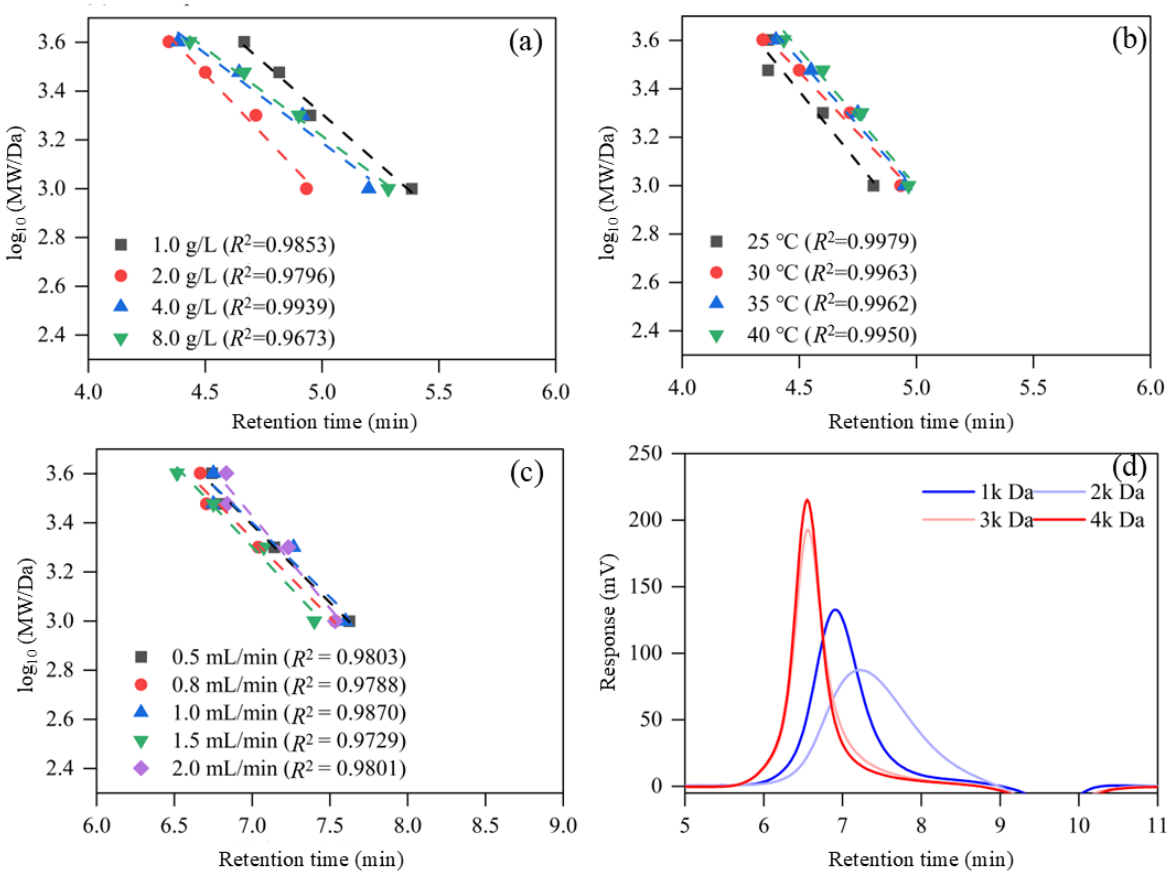

Fig. S5. SEC paramter optimization using the HW-40S column: (a) effect of phosphate mobile phase (ionic strength); (b) effect of column temperature; (c) effect of flow rate; (d) optimized calibration curves obtained with PEG standards.

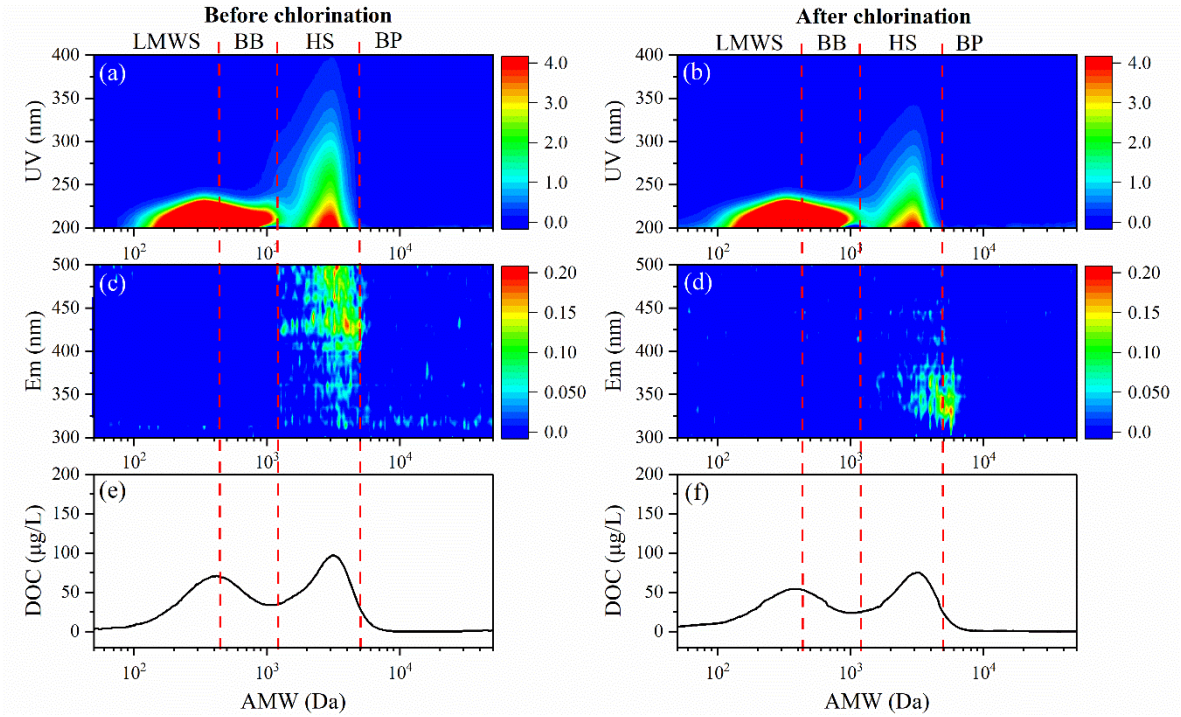

Fig. S6. SEC-DAD-FLD-OCD chromatograms of RW2 before and after 72 h chlorination with 10 mg/L Cl_2: (a,b) UV-Vis absorbance spectra; (c,d) fluorescence spectra; (e,f) SEC-OCD chromatogram.

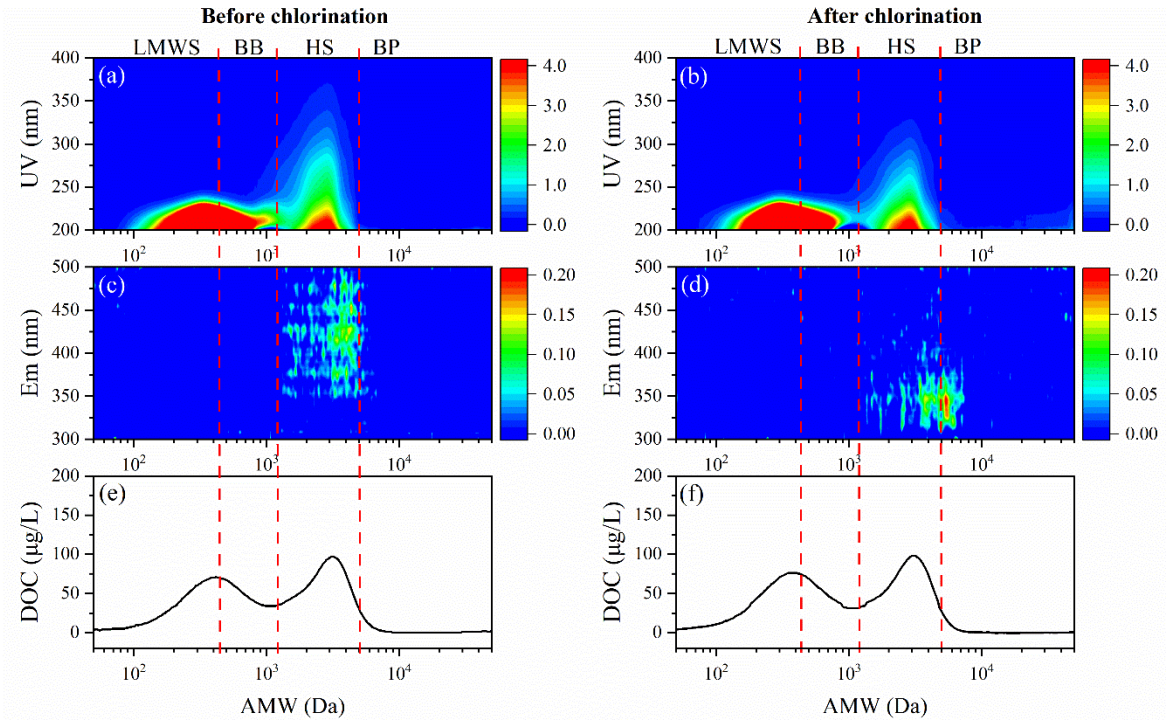

Fig. S7. SEC-DAD-FLD-OCD chromatograms of RW3 before and after 72 h chlorination with 10 mg/L as Cl_2: (a,b) UV-Vis absorbance spectra; (c,d) fluorescence spectra; (e,f) SEC-OCD chromatogram.