Supplementary Information

Changes in Dissolved Organic Matter during the Treatment Processes of a Drinking Water Plant in Sweden and Formation of Previously Unknown Disinfection Byproducts

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Summary

spectrum	Figure	NS	AQ [s]	D1 [s]	WDW2	PR2
^{1}H NMR before / after Cl	6	512	5	5	EM	1
^{13}C NMR before / after Cl	S2	9361 / 9456	1	19	EM	35 (2)
DEPT 45/135 ^{13}C NMR before / after Cl	S2	16384	1	2	EM	12.5
DEPT 90 ^{13}C NMR before / after Cl	S2	32768	1	2	EM	12.5

Table S1: Acquisition parameters of NMR spectra, shown according to figures. NS: number of scans (for 2D NMR: F2); AQ: acquisition time [ms]; D1: relaxation delay [ms]; NE: number of F1 increments in 2D NMR spectra; WDW1, WDW2: apodization functions in F1/ F2 (EM: line broadening factor [Hz]; PR2: coefficients used for windowing functions WDW2.

δ(^{1}H) [ppm]	10 - 7.0	7.0 - 5.3	4.9 - 3.1	3.1 - 1.9	1.9 - 0.0	$H_{olefinic}$ / $H_{aromatic}$	10 - 5.3 (**H**C_{sp^2})
key substructures	**H**$_{ar}$	**H**C=C, **H**CO_2	**H**CO	**H**C-N, **H**C-C-X	**H**C-C-C-		
before Cl	2.4	2.1	19.2	28.7	47.6	0.9	4.5
after Cl	3.0	2.7	19.3	29.1	46.0	0.9	5.7

Table S2: ^{1}H NMR section integrals (percent of non-exchangeable protons) and key substructures of DOM before and after chlorination.

$\delta(^{13}C)$ ppm	220-187	187-167	167-145	145-108	108-90	90-47	47-0	H/C ratio	O/C ratio
Key substructures	**C**=O	**C**OX	$\underline{C}_{ar}$-O	$\underline{C}_{ar}$-C,H	$O_2\underline{C}H$	O**C**H	C**C**H		
before chlorination	1.8	9.8	3.9	8.4	5.6	33.7	36.8	**1.31**	**0.70**
after chlorination	1.7	9.1	3.8	10.8	5.6	32.1	35.5	**1.28**	**0.67**
NMR mixing model	**C=O**	**COOH**	**C_{ar}-O**	**C_{ar}-H**	**O_2CH**	**OCH**	**CH_2**		
H/C ratio	**0**	**1**	**0**	**1**	**1**	**1**	**2**		
O/C ratio	**1**	**2**	**1**	**0**	**2**	**1**	**0**		

DOM (depth)	**CH total**	**CH_2 total**	**CH_3 total**	**ratio (d_1 / c_1 / b_1 / a_1) $H\underline{C}_{ar}$-C / O-H$\underline{C}$-O / H$\underline{C}$-O / H$\underline{C}$-C**	**ratio (b_2 / a_2) $H_2\underline{C}$-O / $H_2\underline{C}$-C**	**ratio (b_3 / a_3) $H_3\underline{C}$-O / $H_3\underline{C}$-C**
before chlorination	36	30	34	15.9 / 1.0 / 33.9 / 49.1	6.8 / 93.2	9.1 / 90.9
after chlorination	35	33	32	14.8 / 1.4 / 34.5 / 49.3	10.7 / 89.3	5.7 / 94.3*

Table S3. (Top): ^{13}C NMR section integrals (percent of total carbon) and key substructures of DOM before and after chlorination. Middle: Substructures used for NMR-derived reverse mixing model with nominal H/C and O/C ratios given. Bottom: percentage of methin, methylene and methyl carbon related to total protonated ^{13}C NMR integral as derived from ^{13}C DEPT NMR spectra of DOM according to carbon multiplicity (left 3 columns) and relative proportions of these CH_n units binding to oxygen versus carbon chemical environments.

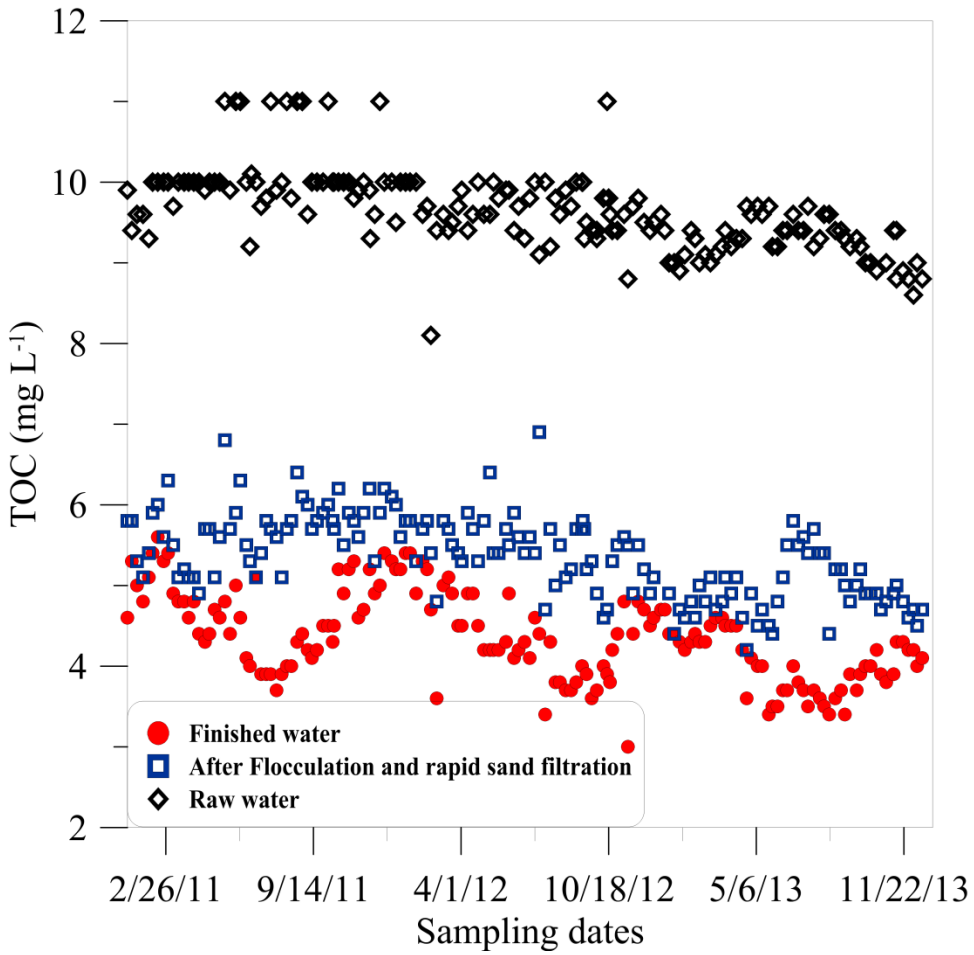

Figure S1: Total organic carbon concentration of the raw water, after flocculation/rapid sand filtration, and of the processed water, Råberga drinking water treatment plant, Linköping, Sweden.

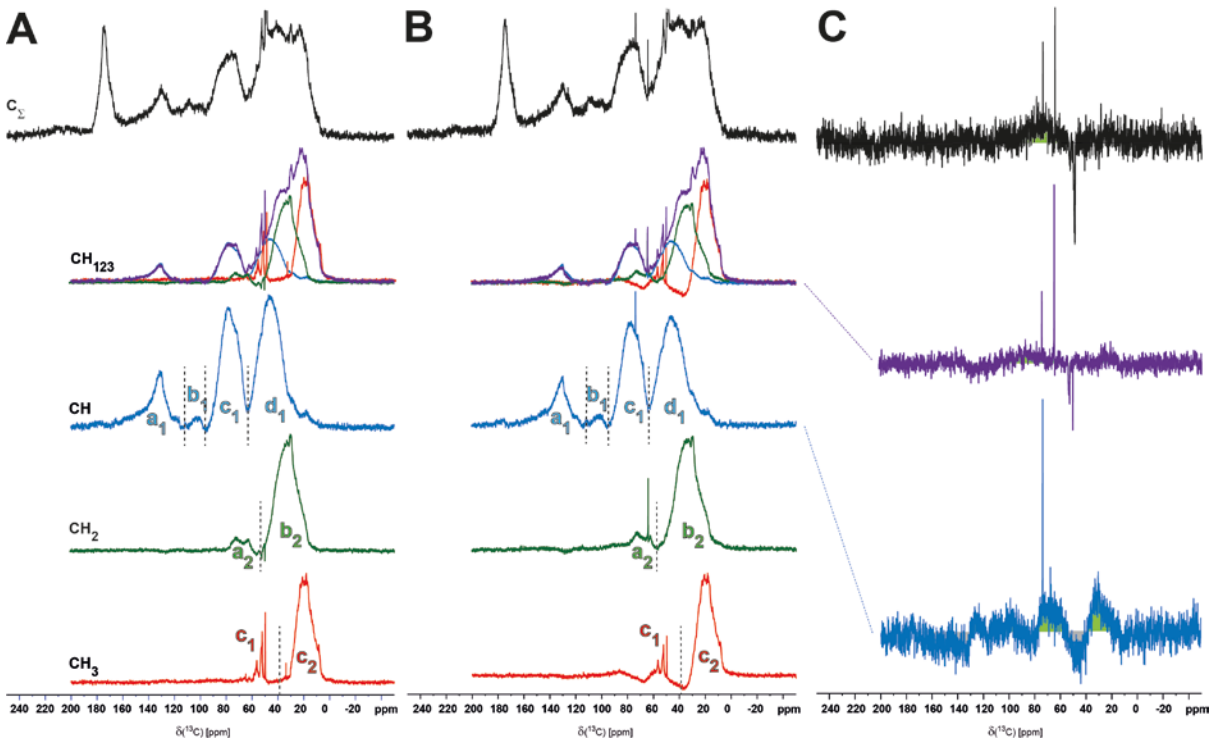

Figure S2: ^{13}C NMR spectra of Raberga slow sand SPE-DOM ($^{12}CD_3OD$ solution, B_0 = 11.7 T) obtained by solid phase extraction (PPL) before (**A**) and after (**B**) chlorination; ^{13}C DEPT NMR spectra: (top) superimposed protonated carbon NMR resonances (CH_{123}; DEPT-45 ^{13}C NMR spectra), multiplicity-edited ^{13}C NMR spectra are (second from top) CH; methin, with indices a_1-d_1 denoting following chemical environments: H**C**$_{ar}$-C / O-H**C**-O / H**C**-O / H**C**-C), (second from bottom) CH_2; methylene, with indices a_2 and b_2 denoting following chemical environments: H_2**C**-O / H_2**C**-**C**, and (bottom) CH_3; methyl, with indices a_3 and b_3 denoting following chemical environments : H_3**C**-O / H_3**C**-C**.** The respective ^{13}C NMR section integrals are provided in Tab. 4. (**C**) difference ^{13}C NMR spectra as derived from (top) single pulse ^{13}C NMR spectra, (middle) DEPT-45 ^{13}C NMR spectra, and (bottom) DEPT-90 ^{13}C NMR spectra.