

Supplementary Information for:

Trihalomethane, Dihaloacetonitrile, and Total *N*-nitrosamine Precursor Adsorption by
Carbon Nanotubes: The Importance of Surface Oxides and Pore Volume

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Supplementary Information contains: Methods; PARAFAC Analysis; Carbon Spectra
Deconvolutions; Model Verification and Permutations; Modeling CNT Wall Type;
Removal of PARAFAC Components; PARAFAC Component Correlations; UV₂₅₄ as a
DBP Precursor Surrogate; References; 21 pages, 7 tables and 9 figures

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53 **Methods**

54 Dissolved organic carbon was measured for each filtered sample using a GE
55 5310C TOC analyzer. Anion concentrations were measured for both BL-RAW and WS-
56 EFF raw waters using a Metrohm 850 Ion Chromatograph with conductivity and UV
57 detectors. Fluorescence EEMs were collected using a dual monochromator fluorescence
58 detector (Agilent Technologies, Model G1321A). Wavelengths used were 250 to 400 nm
59 for excitation and 270 to 600 nm for emission, both in 1 nm increments. A five-point
60 standard curve of quinine sulfate in 0.1 M sulfuric acid was used due to its distinct
61 response at excitation and emission wavelengths of 350 and 450 nm, respectively, and
62 intensity measurements of all spectra were reported in quinine sulfate equivalents.¹
63 Absorbance scans were used to correct for inner-filter effects as suggested by McKnight
64 et al.² and the MATLAB program *Cleanscan*³ was used to correct EEMs for Raleigh and
65 Raman scattering. Values of fluorescence intensity at excitation and emission
66 wavelengths of 345 nm and 425 nm, respectively, are strongly correlated with TTHM
67 precursors⁴ and are shown in Table S1 for both BL-RAW and WS-EFF. Two models
68 were developed using parallel factor (PARAFAC) analysis on arrays of EEMs for each
69 water type to reveal components with distinct excitation-emission signatures and their
70 maximum intensities, F_{MAX} .⁵

71 Disinfection by-product formation potential (DBPFP) of the samples was
72 measured using the procedure detailed in Do et al.⁴ Samples were warmed to room
73 temperature, amended with 20 mM sodium bicarbonate, and adjusted to pH 7.0 using
74 NaOH and/or HCl. Pre-formed 14 g·L⁻¹ as Cl₂ stock monochloramine solution was
75 prepared immediately before chloramination as detailed previously. The stock total

chlorine and monochloramine concentrations were measured on a representative sample volume, following 4,000-6,000 times dilution with Milli-Q water, using Hach powder pillows with a UV-Vis 2450 spectrophotometer (Shimadzu) at wavelengths of 655- and 552 nm, respectively. Samples were dosed with pre-formed monochloramine at 300 mg·L⁻¹ as Cl₂ and stored headspace-free in 1-L chlorine demand free amber glass bottles for 7 days in the dark at room temperature (25 °C ± 2 °C). Following the hold time, the monochloramine and total chlorine residuals were measured and quenched with 20.1 g of a salt mixture (mass ratio of 0.9 g ascorbic acid (C₆H₈O₆): 1 g KH₂PO₄: 39 g Na₂HPO₄) added to each 1 L sample to halt DBP formation reactions as recommended by Kristiana et al.⁶ Total trihalomethanes (TTHMs) and dihaloacetonitriles (DHANs) in the West Side wastewater treatment plant effluent (WS-EFF) samples were quantified by GC-ECD using a 9-point standard curve that ranged from 1- to 100 µg·L⁻¹. Similarly, TTHMs and DHANs in the Beaver Lake raw water (BL-RAW) samples were analyzed using a 12-point standard curve that ranged from 0.1- to 100 µg·L⁻¹. Blanks and check standards were run after every group of six samples.

The pH point of zero charge of the carbon nanotubes (CNTs) was not measured because a stable suspension could not be achieved without CNT modification. Sonication of CNTs in pure water was attempted despite the high probability of damage to the CNT structure,⁷ but failed to produce the stable suspension necessary for zeta potential measurements.

PARAFAC Analysis

EEMs were analyzed by PARAFAC to further characterize the dissolved organic matter and help generalize the precursor surrogate findings. Given the differences in the water types, separate PARAFAC models were used for BL-RAW and WS-EFF samples, each originally consisting of 57 EEMs. Two outliers were removed from the BL-RAW data set while no outliers were found in WS-EFF samples. Split-half analyses showed that BL-RAW samples could be adequately described by a two- or four-component model and the WS-EFF samples could be described by a two- or three-component model. Models with the greatest number of components (i.e., four components for BL-RAW and three components for WS-EFF) were chosen to explain the data because they had the smallest sum of squared errors (Figure S8).

XPS Data Analysis

Binding energy scales were charge corrected using a C1s peak position of 284.4 eV.^{8,9} C1s peaks were deconvoluted with a Gaussian-Lorentzian mix function, allowed to range from 70-80% Gaussian distribution, and a Shirley background subtraction.^{9,10} An asymmetry parameter of 0.19 was applied to the peak representing carbon-carbon bonds;⁸ other bonds assigned were alcohols (C-O), carbonyls (C=O), and carboxyls (COO) with an additional peak fitted to the shake-up features satellite located in the higher binding energy region. Peak locations chosen for the carbon spectra deconvolutions were set as allowable ranges based on ranges found in the literature. Actual peak locations were allowed to vary within the set range in order to achieve the best fit determined by the chi-squared value of the model. The asymmetric carbon peak representing all types of carbon-carbon bonding was set to 284.38-285.50 eV.^{8,10-13} Locations of various types of carbon-

oxygen bonds are as follows: alcohol at 286.00-287.53 eV, carbonyl at 286.45-288.03 eV, and carboxyl at 288.39-289.55 eV.^{8, 9, 11-15} Shake-up features associated with π - π^* transitions were fitted at 289.00-291.60 eV.¹¹ Each individual peak was allowed to vary from 70- to 80% Gaussian distribution in order to find the best fit.^{9, 10, 16}

Model Verification and Permutations

Results in Table 2 are based on reasonable assumptions with respect to a normal distribution of residuals and constant error variance. The results of the Wilk-Shapiro test¹⁷ for TTHM ($p = 0.788$), DHAN ($p = 0.066$) and TONO ($p = 0.339$) were all greater than $p = 0.05$; we therefore fail to reject a normal distribution of residuals.

Further investigation of the relationships between physical and chemical characteristics of the nine CNT types through simple linear regressions revealed strong correlations between percent alcohol groups and S_{BET} ($R^2 = 0.95$) and CPV ($R^2 = 0.90$). Multiple linear regression models of surface oxide groups and physical characteristics showed that alcohol groups were significant to S_{BET} and CPV when controlling for carbonyl and carboxyl groups. These findings show that multicollinearity of alcohol groups and physical properties results in variance inflation factors ($\text{VIF} = (1 - R^2)^{-1}$, where R^2 is relevant to a multiple linear regression model of one independent variable versus the other independent variables) greater than ten, which could make it impossible to observe otherwise significant independent variables in models of DBP ratio. Of the physical and chemical characteristics, carboxyl groups suffer least from variance inflation ($\text{VIF} = 1.27$), and it is possible that this variable serves as a surrogate for significance of physical characteristics. To further study possible significance of alcohol groups in the face of multicollinearity, the carbonyl groups variable, which was insignificant in all

models, was deleted from models of TTHM and DHAN Ratios. This deletion revealed negative significance of alcohol groups to DHAN ratio, indicating that an increase in alcohol groups improved removal of DHAN precursors.

As further evidence of multicollinearity, linear regression between S_{BET} and CPV variables also results in a very strong correlation ($R^2 = 0.97$). However, in the multivariate analysis including both physical variables, only CPV was significant to changes in DBPFP Ratio when controlling for surface area. The same cannot be said of S_{BET} when controlling for CPV. As the multivariate model is capable of providing a more comprehensive assessment of the significance of variables than simple linear regression of variable pairs, it is reasonable to conclude that CPV is a more relevant variable to discuss than S_{BET} in terms of relationships to chemical characteristics and DBPFP Ratio. Nevertheless, Figure S4 shows the linear regressions for the wavelength pair associated with the maximum R^2 value for TTHM ($I_{369/365}$) and DHAN ($I_{379/356}$). Samples were included regardless of DBP type (TTHM and DHAN only) or source water and an aggregate R^2 value of 0.91 indicates that fluorescence measurements can be used as a reliable surrogate of organic precursor concentrations for TTHM and DHAN. As detailed in the SI, UV_{254} was also assessed as a DBP surrogate, but lacked sensitivity at low absorbance values (less than 0.05 cm^{-1}).

Modeling CNT Wall Type

Of the nine types of CNTs studied, two are single-walled (SWCNTs) and seven are multi-walled (MWCNTs). To explore the effects of these designations, a binary variable was added to the model to distinguish between SWCNTs and MWCNTs in addition to their physical and chemical characteristics (Table 1). This binary variable was

significant in both TTHM and DHAN models and showed that DBP ratios were significantly smaller in SWCNT-treated waters (i.e., SWCNTs adsorbed more TTHM and DHAN precursors). Also, controlling for the new binary variable, CPV had negative, significant effects on DBP ratio for DHAN in general ($n = 36$) and for TTHM in WS-EFF only ($n = 18$). However, without more observations of SWCNT types and/or greater chemical and physical detail to distinguish between single- and multi-walled CNTs, this study does not focus on the general difference in CNT wall type and its relationship to other variables.

Removal of PARAFAC Components

The maxima locations of PARAFAC Components 1 and 3 in BL-RAW (Figures S5A and S5C) and WS-EFF (Figures S6A and S6C) corresponded to locations previously characterized as humic- and fulvic-like fluorophores.¹⁸ Similarly, the maxima locations of Component 2 corresponded to protein-like fluorophores for BL-RAW (Figure S5B) and WS-EFF (Figure S6B).¹⁹ Component 4 in the BL-RAW model was considered negligible due to its location at maximum emission wavelengths and its low F_{MAX} values, which were insensitive to treatment. To gain further insight into the DBP precursors represented by each PARAFAC component and their removal by the nine types of CNTs, mean percent removals were calculated for each component (Table S6) based on F_{MAX} values for BL-RAW and WS-EFF (Table S5).

Using all nine possible combinations of triplicate samples for both raw and treated waters for a given CNT type, a conservatively large range of percent removal values were determined and used to calculate mean removals and 95% confidence intervals using the t-distribution (Table S5) due to small sample estimates of standard deviation. Removal of

Components 1, 2 and 3 in WS-EFF by the CNTs all show similar trends in CNT performance to those observed for the removal of total THM formation potential (TTHMFP) and dihaloacetonitrile formation potential (DHANFP) (Figure S7A and S7B). Additionally, removal of Components 1 and 3 show strong correlations to DBPFP in BL-RAW (Figure S7D and S7E). Weak correlations were observed for total *N*-nitrosamine (TONO) formation potential removal (Figure S7C) and Components 2 and 4 in BL-RAW. For all nine CNT types in WS-EFF, Component 2 (protein-like fluorophores) had the highest mean percent removal (32-80%) of the three components. For six CNT types in BL-RAW, negative mean percent removals were calculated for Component 2, which was attributed to a combination of low concentrations of protein-like compounds in BL-RAW source water and interferences of humic- and fulvic-like fluorophores skewing the magnitude of the fluorescent response, similar to the findings of others.²⁰ Additionally, the samples with negative mean percent removals also have relatively large 95% confidence intervals (12-339%). These observations illustrated the need for further investigation into the independence of individual PARAFAC components.

PARAFAC Component Correlations

Linear associations between PARAFAC components were tested for data sets incorporating samples treated with both low and high doses of CNTs. Correlations may be considered “weak” if $R < 0.5$, “strong” if $R > 0.8$, and “moderate” otherwise.²¹ As shown in Table S7 for the BL-RAW samples, the correlation is strong between Components 1 and 3 and moderate between Component 1 and Components 2 and 4. In contrast, correlations among Components 2, 3, and 4 are weak with *R* values between 0.43-0.49. For the WS-EFF samples, all correlations were strong between the three

components, with R values of 0.85, 0.94, and 0.97. As such, even if protein-like fluorophore groups were the predominant precursors of TONO, the influence of humic- and fulvic-like fluorophores would obscure this finding and produce poor correlations such as those observed in Figure S7C.

UV₂₅₄ as a DBP Precursor Surrogate

Performing selected linear comparisons between single dependent variables and DBPFP revealed an interesting relationship between UV₂₅₄ and TTHMFP (Figure S9A) and DHANFP (Figure S9B). While strong linear correlations existed between UV₂₅₄ for the WS-EFF samples (TTHMFP, $R^2 = 0.74$ and DHANFP, $R^2 = 0.78$), those for BL-RAW samples had R^2 values less than 0.01, indicating the sensitivity of the absorbance scans were insufficient for characterization of TTHM and DHAN precursors. The sensitivity of UV₂₅₄ measurements could possibly be improved by utilizing a 5 cm pathlength cuvette, instead of the 1-cm cuvette used in this study. However, fluorescence measurements utilize a much smaller pathlength of 0.5 mm while still maintaining a comparatively high sensitivity. This in addition to its usefulness across multiple water types (Figure S4) indicates fluorescence is a more robust DBP precursor surrogate than UV₂₅₄.

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269 **Table S1.** Raw Water Characteristics

Water Type	BL-RAW¹	WS-EFF²
pH	7.82	7.93
DOC ³ (mg·L ⁻¹)	2.33	5.98
UV ₂₅₄ (cm ⁻¹)	0.034	0.096
I _{345/425} (QSE) ⁴	5.16	14.25
Specific Conductivity (μS·cm ⁻¹)	155	535
Fluoride (mg·L ⁻¹)	0.11	0.47
Chloride (mg·L ⁻¹)	4.1	47.9
Bromide (mg·L ⁻¹)	0.11	0.16
Nitrate (mg·L ⁻¹)	1.3	23.9
Phosphate (mg·L ⁻¹)	ND ⁵	0.29
Sulfate (mg·L ⁻¹)	8.0	47.2
Nitrite (mg·L ⁻¹)	ND	ND
¹ Raw intake water from Beaver Lake collected on July 7, 2014		
² Effluent from the West Side Wastewater Treatment Plant collected on June 3, 2014		
³ Dissolved Organic Carbon		
⁴ Average fluorescence intensity at excitation and emission wavelengths of 325 nm and 425 nm respectively		
⁵ Not detected		

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Table S2. Manufacturer-specified properties of the selected carbon nanotubes.

CNT ¹ Number	CNT Type	Supplier Description	Diameter (nm)	Length (mm)	S _{BET} ² (m ² g ⁻¹)	Supplier
1	SW ³	SWNTs (90%, regular length)	1-2	5-30	300-380	NAM, Inc. ⁴
2	MW ⁵	SW-DW CNTs 60	0.8-1.6	5-30	407	Cheap Tubes, Inc.
3		C-Grade MWNTs	1-3	80-150	NA ⁶	NanoTechLabs, Inc.
4		MW CNTs 8 nm	2-5	10-30	500	Cheap Tubes, Inc.
5		MW CNTs 20-30 nm	5-10	10-30	110	Cheap Tubes, Inc.
6		95%, OD/ID: <10/2-7 nm	2-7	5-15	40-600	NAM, Inc.
7		95%, OD/ID: 30-50/5-15 nm	5-15	10-20	90-120	NAM, Inc.
8		PD30L5-20	15-45	5-20	200-400	NanoLab, Inc.
9		PD30L1-5	15-45	1-5	200-400	NanoLab, Inc.

¹Carbon nanotube

²Supplier provided specific surface area from nitrogen adsorption isotherms using the Brunauer-Emmett-Teller (BET) model

³Single-walled

⁴Nanostructured & Amorphous Materials, Inc.

⁵Multi-walled

⁶Not Available

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280 **Table S3.** Preliminary DBPFP Removal Testing

CNT Dose (mg L ⁻¹) ¹	Water Type ²	Average TTHMFP ³ Removal (%)	Average DHANFP ⁴ Removal (%)
0	BL-RAW	-	-
5	BL-RAW	14	-
50	BL-RAW	51	-
520	BL-RAW	98	-
0	BL-RAW	-	-
5	BL-RAW	26	37
50	BL-RAW	71	94
0	WS-EFF	-	-
5	WS-EFF	11	20
50	WS-EFF	67	96

¹Single-walled CNTs were used in all dosed samples²Beaver Lake raw water (BL-RAW) was collected on August 15, 2013 for first set of samples and April 5, 2014 for the second set. West Side WWTP effluent (WS-EFF) was collected on April 9, 2014.³Average total trihalomethane formation potential based on duplicate samples⁴Average dichloroacetonitrile formation potential based on duplicate samples

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Table S4. Chlorine Residuals following filtration in batch studies

CNT Type	CNT Dose (mg•L ⁻¹)	Average Chlorine Residual (mg•L ⁻¹)	
		BL-RAW	WS-EFF
Blank	0	9.29	9.26
1	25	11.30	10.27
	50	11.47	10.18
2	25	13.83	11.32
	50	14.47	11.23
3	25	14.63	12.77
	50	14.90	12.31
4	25	14.09	12.03
	50	14.85	12.37
5	25	14.35	12.40
	50	14.22	10.72
6	25	15.30	12.65
	50	15.23	13.50
7	25	13.19	12.43
	50	14.00	13.18
8	25	14.76	11.20
	50	15.37	10.49
9	25	11.94	11.48
	50	13.80	10.80

286 **Table S5.** Fluorescence maximum (F_{MAX}) values

CNT Type	CNT Dose (mg L ⁻¹)	Water Type						
		BL-RAW				WS-EFF		
		C1	C2	C3	C4	C1	C2	C3
Blank	0	9.7	5.1	3.0	1.8	17.1	10.1	9.5
		9.9	4.9	3.1	1.8	18.2	11.0	12.5
		9.9	4.3	3.0	1.8	18.0	10.9	12.1
1	25	4.2	1.9	1.1	1.5	8.1	3.5	4.8
		4.2	1.9	1.2	1.6	8.1	3.4	5.0
		4.3	2.0	1.2	1.4	8.4	3.6	5.8
	50	3.2	1.5	0.9	1.6	5.6	2.2	4.0
		3.2	1.5	0.9	1.3	5.6	2.2	4.4
		3.6	1.9	0.9	1.6	5.4	2.1	5.0
2	25	4.7	2.1	1.6	1.5	7.4	4.0	4.0
		4.9	2.1	1.6	1.5	7.5	4.1	4.2
		4.6	2.2	1.5	1.4	7.5	4.1	4.4
	50	3.2	1.6	1.0	1.3	4.4	2.3	2.6
		1.8	1.4	1.0	1.7	4.4	2.3	2.6
		4.0	3.2	1.6	1.7	4.5	2.4	2.9
3	25	8.0	6.5	2.3	2.4	13.1	6.4	9.4
		8.2	8.1	2.2	1.8	13.0	6.2	9.2
		7.8	4.5	2.2	1.8	13.6	6.5	10.1
	50	7.2	6.6	2.1	2.7	10.1	4.2	7.9
		5.2	2.0	1.6	1.6	9.9	4.0	6.8
		7.2	4.0	1.9	1.8	10.0	4.1	7.6
4	25	5.5	3.9	1.6	1.8	8.9	3.5	6.3
		5.6	6.0	1.6	2.0	7.8	3.1	4.7
		5.5	3.8	1.6	1.9	8.3	3.4	6.1
	50	4.2	3.2	1.2	1.6	5.5	2.1	3.9
		4.0	3.5	1.3	1.8	5.6	2.2	4.3
		4.1	3.3	1.2	1.7	5.7	2.2	4.4
5	25	6.1	6.9	1.9	1.8	10.9	4.8	8.2
		6.6	6.9	2.0	1.7	10.8	4.8	7.7
		6.7	9.9	2.0	1.8	11.1	5.0	9.1
	50	4.7	2.8	1.4	1.6	7.8	3.1	6.3
		5.5	4.9	1.7	1.8	7.9	3.2	6.2
		5.0	3.5	1.4	1.8	7.5	3.0	5.1
6	25	6.8	15.3	1.9	1.9	9.2	3.8	6.7
		6.7	13.3	1.9	1.9	9.2	3.9	6.4
		7.4	7.7	2.1	2.2	9.5	3.9	6.5

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289 **Table S5 Continued.**

CNT Type	CNT Dose (mg L ⁻¹)	Water Type						
		BL-RAW				WS-EFF		
		C1	C2	C3	C4	C1	C2	C3
6	50	4.9	3.0	1.3	1.8	6.7	2.5	5.3
		-	-	-	-	6.2	2.4	4.2
		5.6	14.3	1.5	1.8	6.6	2.5	5.3
7	25	9.5	10.5	2.7	2.0	14.2	7.1	10.7
		10.2	11.1	2.9	2.0	14.1	7.2	10.7
		7.9	5.2	2.3	1.9	14.1	7.3	10.9
	50	7.8	17.6	2.1	2.0	11.6	5.1	10.5
		6.7	9.8	2.0	1.9	11.6	5.2	9.0
		8.9	10.8	2.2	2.3	11.7	5.3	9.2
8	25	-	-	-	-	8.9	3.4	7.1
		6.5	7.3	1.7	2.1	9.2	3.6	7.5
		6.1	10.7	1.7	1.7	10.1	3.9	8.4
	50	4.7	8.0	1.5	1.7	6.7	2.5	5.8
		3.7	3.4	1.2	1.4	6.6	2.3	7.4
		4.5	10.0	1.3	1.6	6.5	2.4	5.3
9	25	5.7	8.6	1.5	1.7	9.7	4.0	7.4
		5.5	6.2	1.6	1.7	9.4	3.9	7.1
		5.6	6.8	1.8	2.3	9.5	3.8	7.8
	50	4.7	8.5	1.4	1.7	6.5	2.4	4.8
		4.1	7.5	1.3	2.1	6.6	2.4	5.0
		4.5	4.1	1.4	1.6	6.6	2.5	5.2

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292 **Table S6.** Mean percent removal of each PARAFAC component

Water Type	CNT Type	Dose = 25 mg/L CNTs			
		C1 ¹	C2	C3	C4
BL-RAW	1	57 ± 2.5 ²	59 ± 11	62 ± 2.3	16 ± 16
	2	52 ± 5.0	55 ± 14	48 ± 6.3	19 ± 7.8
	3	19 ± 8.4	-37 ± 123	27 ± 6.1	-11 ± 48
	4	44 ± 2.3	2 ± 89	47 ± 2.6	-7 ± 12
	5	34 ± 10	-70 ± 129	36 ± 7.2	2 ± 5.6
	6	29 ± 12	-160 ± 252	35 ± 13	-11 ± 30
	7	6 ± 33	-92 ± 200	12 ± 27	-9 ± 14
	8	36 ± 7.1	-93 ± 129	44 ± 2.6	-5 ± 28
	9	43 ± 4.0	-53 ± 102	46 ± 10	-5 ± 55
WS-EFF	1	54 ± 6.2	67 ± 5.4	53 ± 30	- ³
	2	58 ± 4.1	62 ± 5.5	62 ± 18	-
	3	25 ± 10.9	40 ± 11	14 ± 43	-
	4	53 ± 11.3	69 ± 7.5	49 ± 35	-
	5	38 ± 7.6	54 ± 8.1	25 ± 43	-
	6	47 ± 6.6	64 ± 5.5	42 ± 25	-
	7	20 ± 7.5	32 ± 10	4 ± 40	-
	8	47 ± 13	66 ± 10	31 ± 42	-
	9	46 ± 6.5	63 ± 6.1	33 ± 33	-

¹Components 1-4 represented as C1-C4

²95% confidence intervals calculated from maximum range of possible removal values

³Model for WS-EFF were only validated with a maximum of three components

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295 **Table S6 Continued.**

Water Type	CNT Type	Dose = 50 mg/L CNTs			
		C1	C2	C3	C4
BL-RAW	1	66 ± 7.5	65 ± 18	70 ± 1.2	15 ± 25
	2	69 ± 30	55 ± 62	60 ± 27	10 ± 32
	3	34 ± 31	8 ± 145	39 ± 21	-12 ± 86
	4	58 ± 3.5	29 ± 21	59 ± 4.9	4 ± 21
	5	49 ± 12	20 ± 76	51 ± 12	2 ± 18
	6	47 ± 11	-89 ± 339	54 ± 9.6	1 ± 3.6
	7	21 ± 31	-175 ± 292	31 ± 14	-16 ± 32
	8	56 ± 15	-54 ± 206	56 ± 14	13 ± 23
	9	55 ± 9.0	-44 ± 145	54 ± 8.0	1 ± 38
WS-EFF	1	69 ± 4.1	80 ± 3.5	60 ± 27	-
	2	75 ± 3.0	78 ± 3.4	75 ± 14	-
	3	44 ± 6.4	61 ± 5.9	33 ± 37	-
	4	68 ± 4.3	80 ± 3.6	62 ± 20	-
	5	56 ± 5.7	71 ± 4.9	47 ± 32	-
	6	63 ± 6.5	77 ± 4.6	56 ± 27	-
	7	34 ± 6.2	51 ± 8.2	14 ± 52	-
	8	63 ± 5.0	77 ± 4.7	44 ± 47	-
	9	63 ± 3.9	77 ± 3.4	55 ± 21	-

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297 **Table S7.** Linear correlations (R) between components of BL-RAW and WS-EFF
 298 PARAFAC Models

Water Type	Components			
		C1	C2	C3
BL-RAW	C2	0.51	-	-
	C3	0.97	0.43	-
	C4	0.54	0.47	0.49
WS-EFF	C2	0.97	-	-
	C3	0.94	0.85	-

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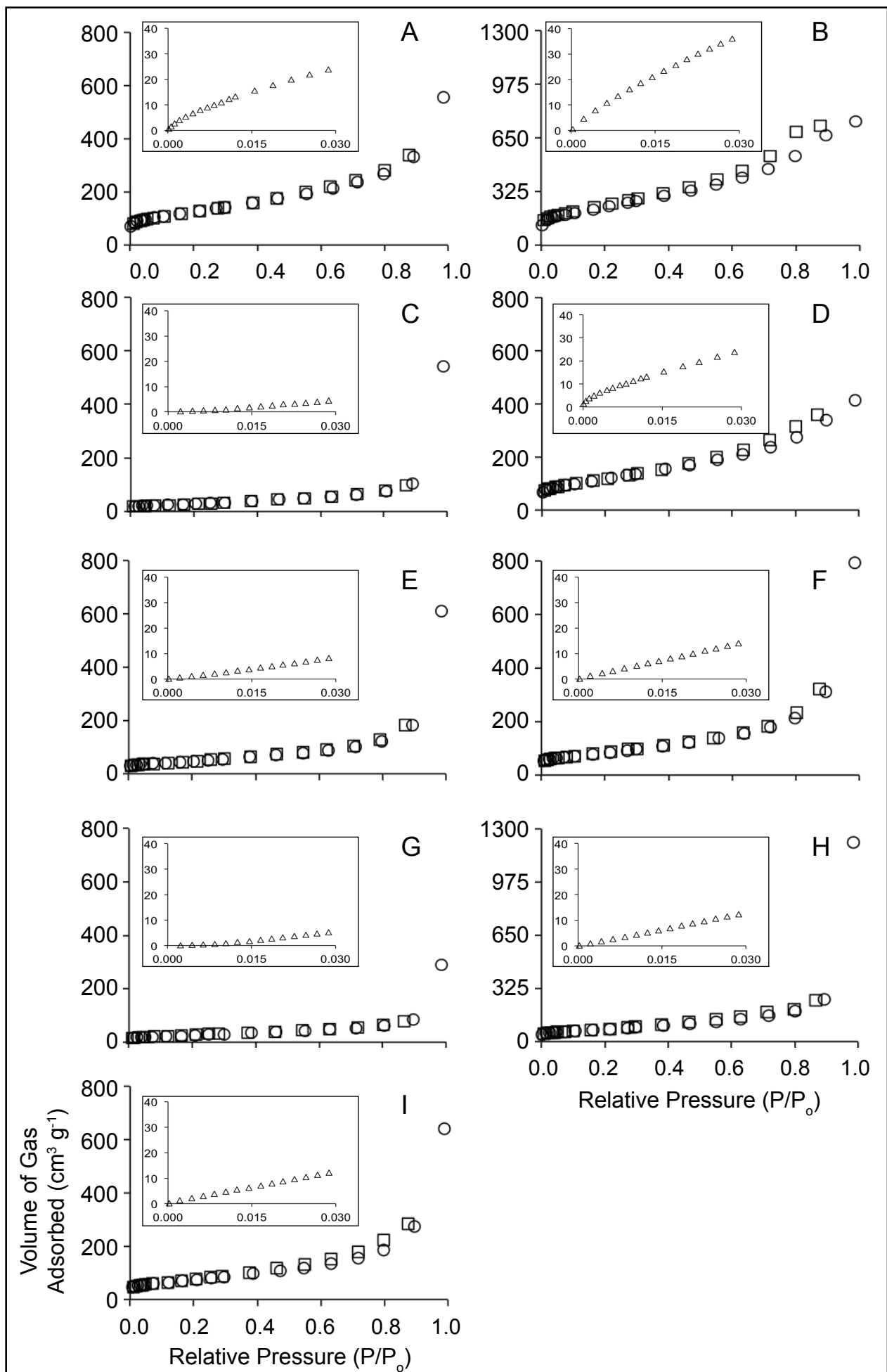


Figure S1. Gas Adsorption Isotherms for CNT Types 1-9 (Figures S1A-S1I). Nitrogen gas adsorption (○) and desorption (□) loops are accompanied by inset carbon dioxide gas adsorption (△) loops. Units are constant for all isotherms.

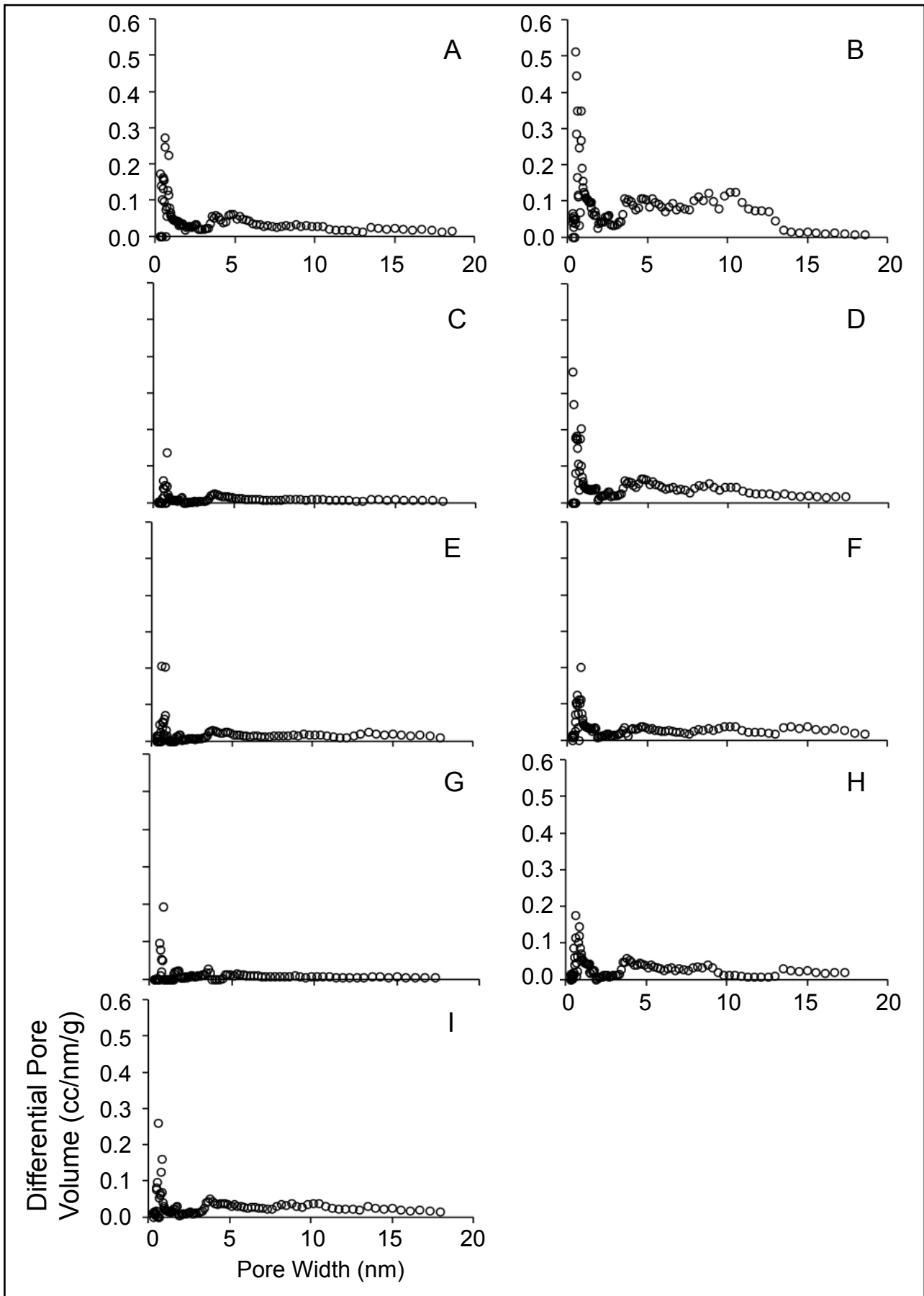


Figure S2. Pore volume distributions for CNT Types 1-9 (Figures S2A-S2I), all with identical scales

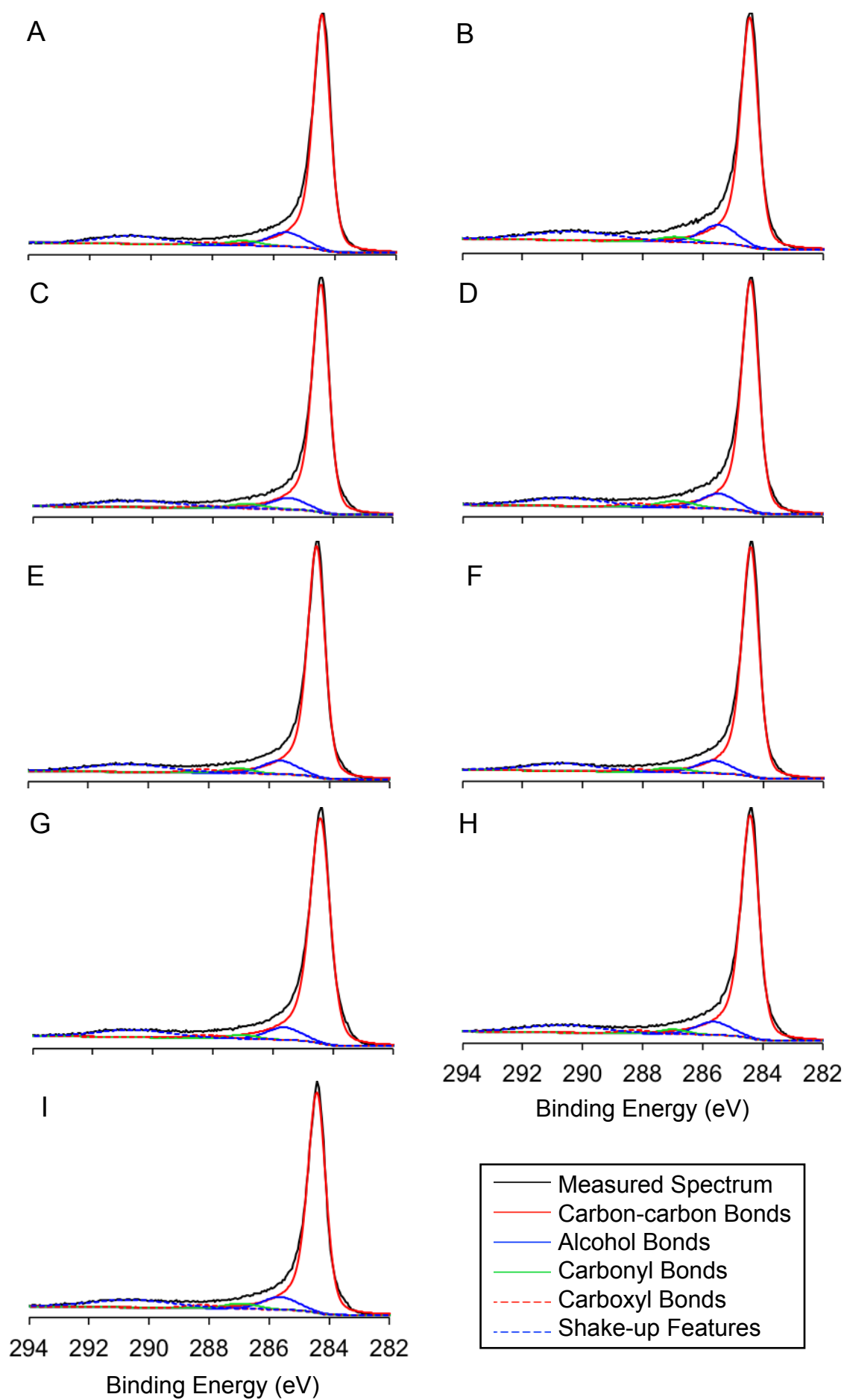


Figure S3. Deconvolutions of Carbon Spectra from XPS Measurements for CNT Types 1-9 (Figures S3A-S3I)

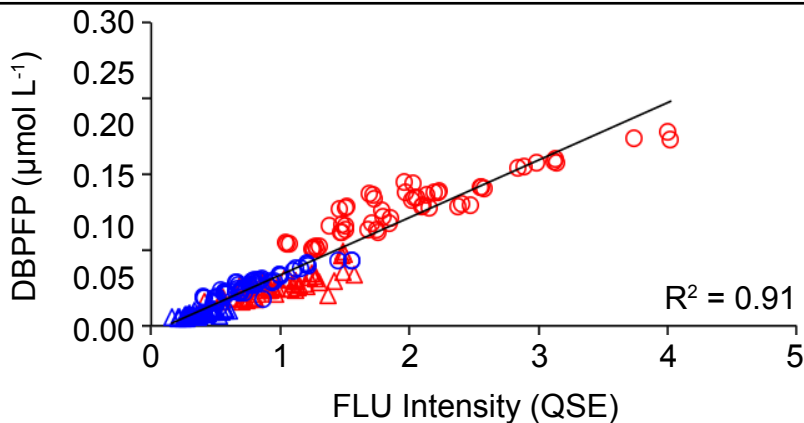


Figure S4. Linear regression of fluorescence at R_{MAX}^2 excitation-emission wavelength pairs against TTHMFP in BL-RAW (\triangle) and WS-EFF (\circ) and DHANFP in BL-RAW (\triangle) and WS-EFF (\circ).

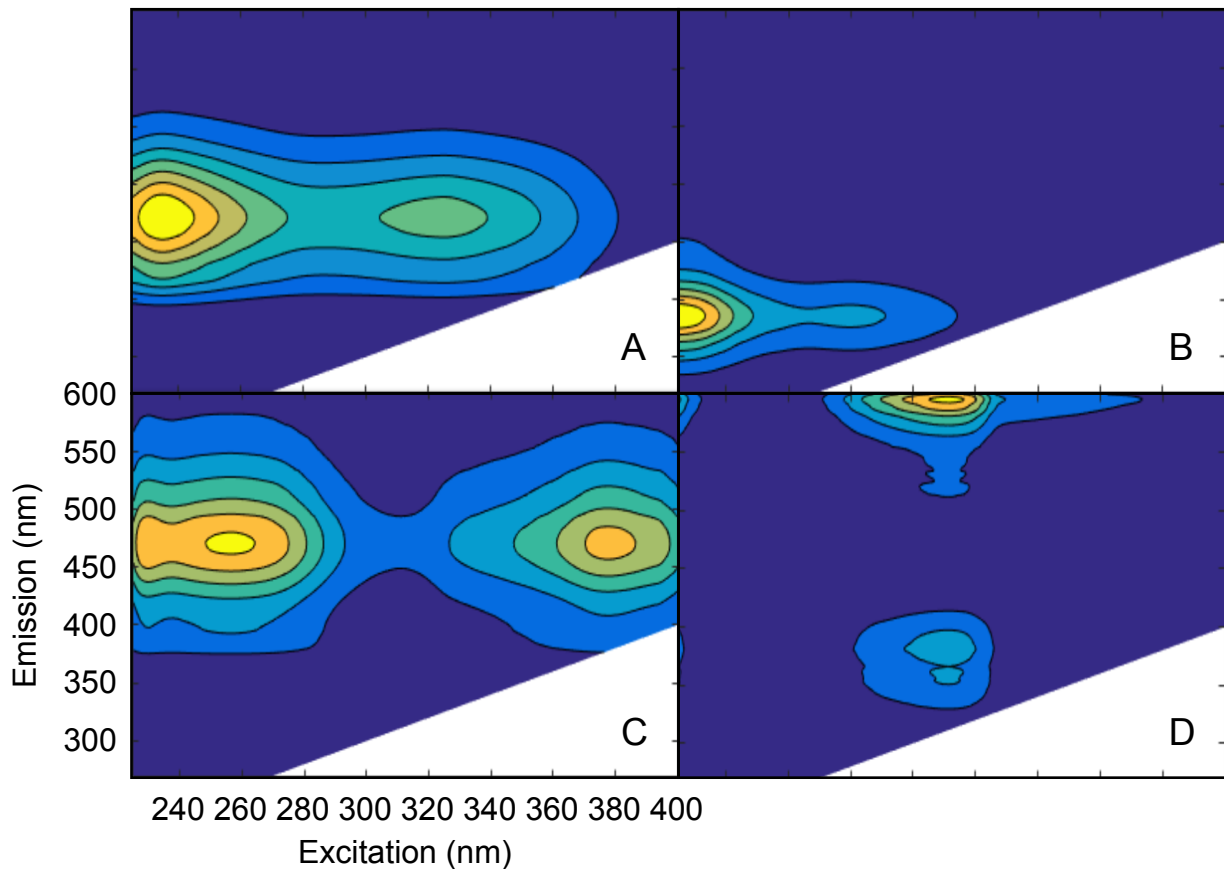


Figure S5. PARAFAC Component EEMs for Beaver Lake Raw Water. A) Component 1, B) Component 2 and D) Component 4 utilize the axes specified in C) Component 3.

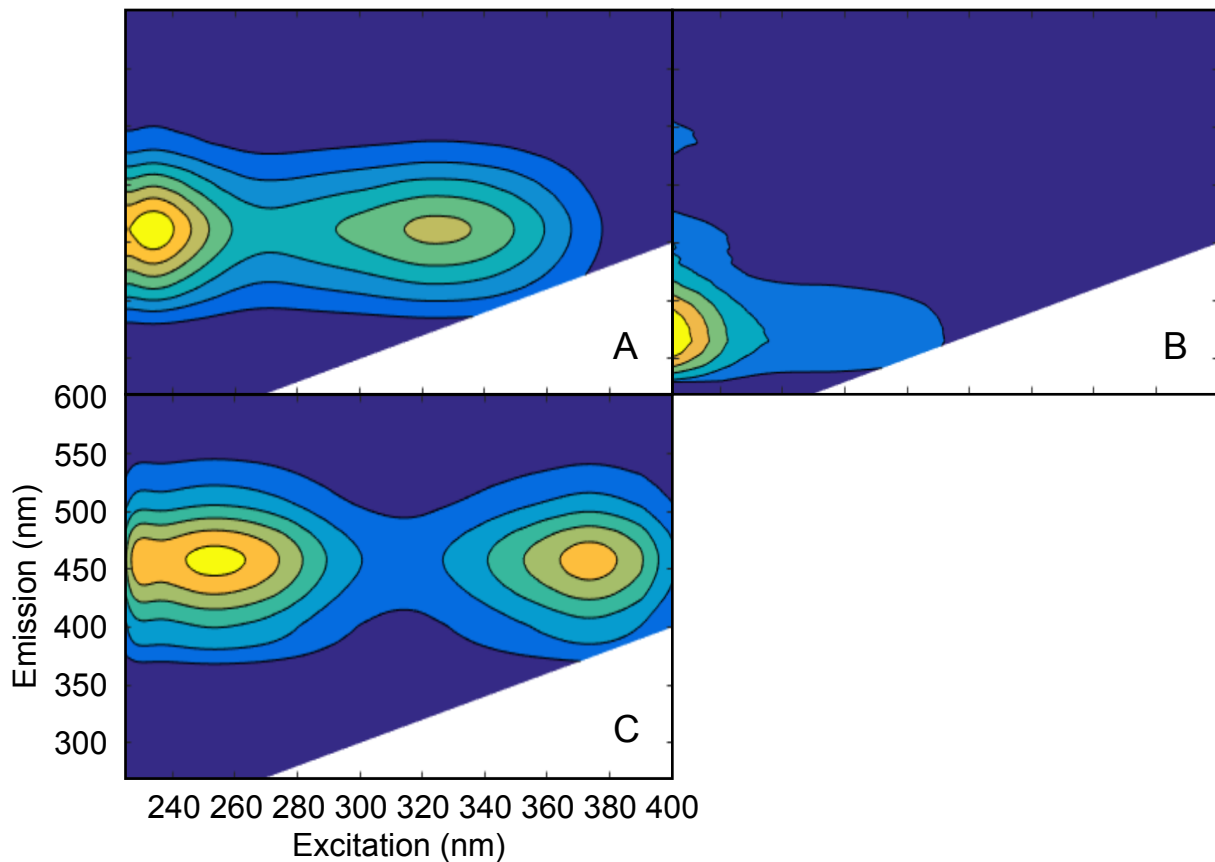


Figure S6. PARAFAC Component EEMs for West Side WWTP Effluent. A) Component 1 and B) Component 2 utilize the axes specified in C) Component 3.

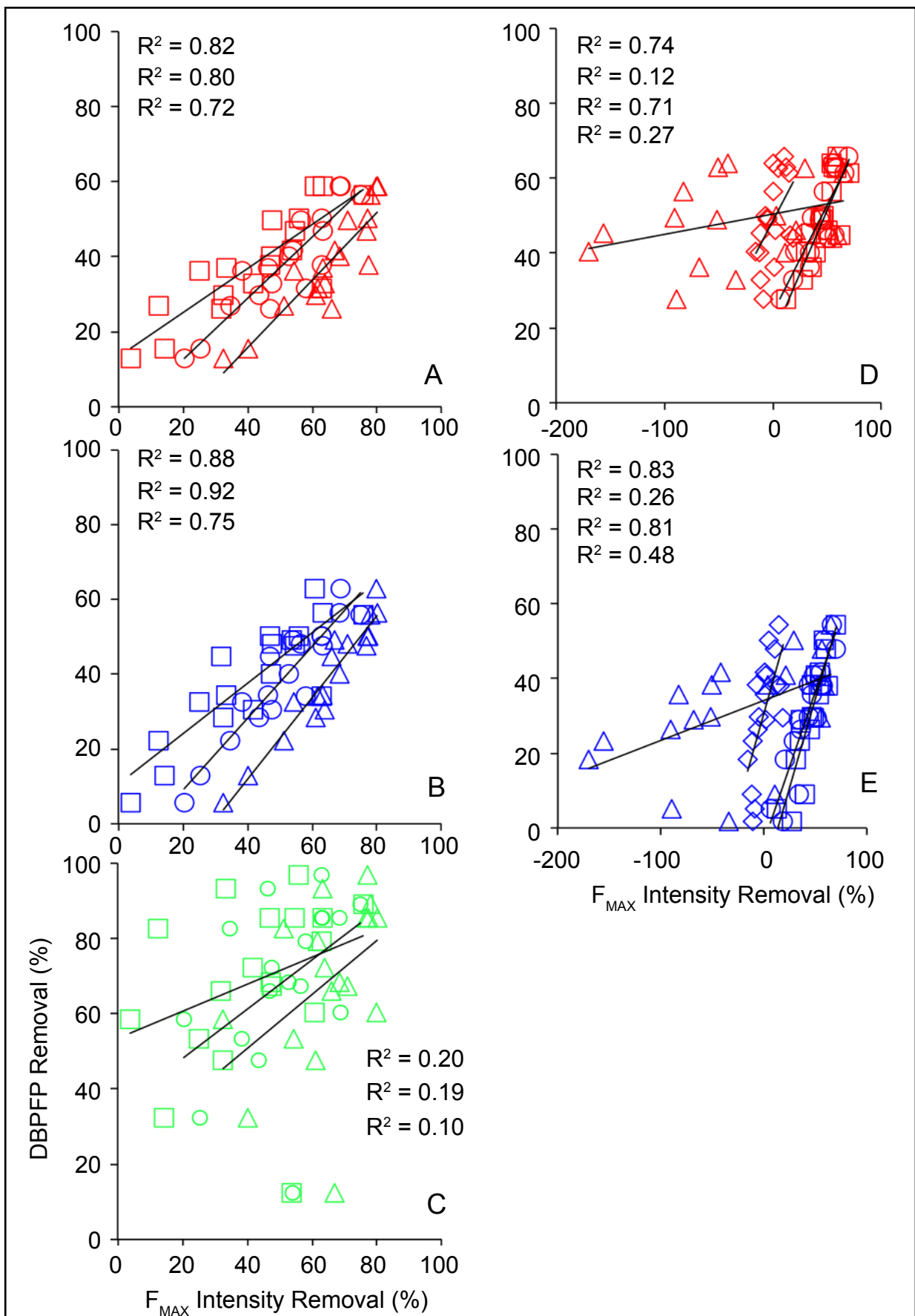


Figure S7. Linear regressions of DBPFP percent removal against percent removal of F_{MAX} of PARAFAC Components 1 (○), 2 (△), 3 (□), and 4 (◇) for TTHMFP, DHANFP, and TONOFP (Figures S8A-S8C) in WS-EFF and TTHMFP and DHANFP (Figures S8D and S8E) in BL-RAW. R^2 values appear according to numerical Component order.

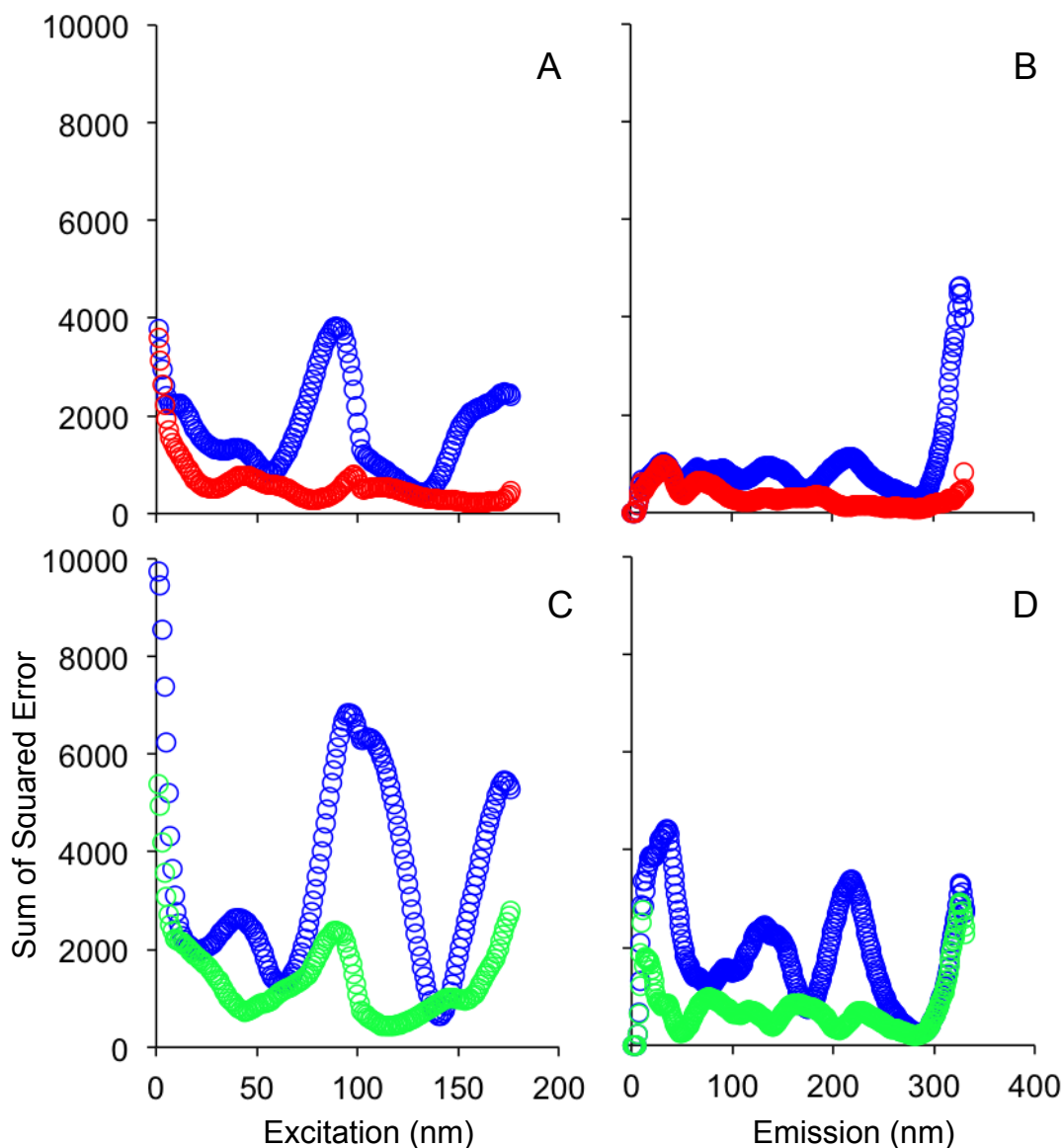


Figure S8. Sum of squared errors for excitation and emission wavelengths based on PARAFAC models with varying quantities of components. Two component (○) and 4 component (○) models were validated for BL-RAW (Figure S9A and S9B). Two component and three component (○) models were validated for WS-EFF (Figure S9C and S9D).

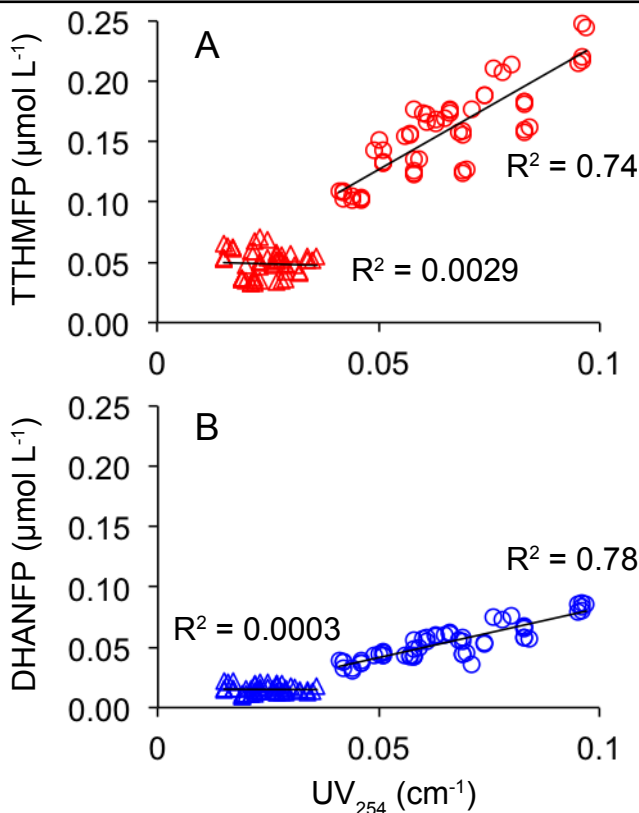


Figure S9. Linear regression of TTHMFP in BL-RAW (○) and WS-EFF (△) (Figure S10A) and DHANFP in BL-RAW (○) and WS-EFF (△) (Figure S10B).