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Dissolved organic matter signatures in urban surface waters: spatio-temporal patterns and drivers

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Table S1: Coordinates, land cover, origin and special features. Longitude is given in decimal degrees East and latitude in decimal degrees North.

Site ID	Site name	Water body type	Latitude	Longitude	Agri-culture (%)	Fo-rest (%)	Urban pave-ment (%)	Urban green space (%)	Origin	Special features
H1	Teltowkanal	River	52.44239	13.32454	0	0	60	30	Artificial	Channelized, WWTP
H2	Teltowkanal	River	52.42642	13.52039	0	0	100	0	Artificial	Channelized, WWTP
H3	Wuhle	Stream	52.52562	13.57913	50	0	50	0	Natural	
H4	Tegeler Fliess	Stream	52.63442	13.38013	50	0	10	40	Natural	
L1	Biesdorfer See	Lake	52.50331	13.5497	0	0	50	50	Artificial	
L2	Obersee	Lake	52.54856	13.48972	0	0	50	50	Artificial	
L3	Ploetzensee	Lake	52.5438	13.33049	0	0	0	100	Natural	
L4	Gross Glienicker	Lake	52.46417	13.11489	0	10	0	90	Natural	
L5	Havel	Lake	52.4431	13.14453	0	0	100	0	Natural	
L6	Schlachtensee	Lake	52.44066	13.21183	0	60	30	10	Natural	
L7	Müggelsee	Lake	52.43837	13.6451	0	70	30	0	Natural	
P1	Hoheheideteic h	Pond	52.57694	13.16428	0	100	0	0	Natural	Protected area
P2	Hamburger Teich	Pond	52.56738	13.44549	0	0	30	70	Artificial	
P3	Ruhwaldteich	Pond	52.52573	13.25998	0	0	50	50	Artificial	
P4	Kienhorstbeck en	Pond	52.57724	13.34556	0	0	0	100	Artificial	Former WWTP runoff input
P5	Mittelfeldteich	Pond	52.61208	13.23045	0	100	0	0	Artificial	Protected area
P6	Neurandteich	Pond	52.63883	13.27377	0	0	65	35	Artificial	

P7	Möwensee	Pond	52.55282	13.33545	0	0	30	70	Artificial	
R1	Müggelspree	River	52.42985	13.68912	0	0	100	0	Natural	Channelized
R2	Landwehrkanal	River	52.51935	13.31959	0	0	80	20	Artificial	Channelized
R3	Spree	River	52.53613	13.21622	0	0	100	0	Natural	Channelized
R4	Kuhlake	River	52.57817	13.16509	0	100	0	0	Natural	Protected area
R5	Neukölln Canal	River	52.48936	13.43949	0	0	30	70	Artificial	Channelized
R6	Spree	River	52.47137	13.49683	0	0	100	0	Natural	Channelized
R7	Panke	River	52.5369	13.36759	0	0	60	40	Natural	Channelized, WWTP (from 2015)
S1	Zingergraben	Stream	52.58209	13.38594	0	0	95	5	Artificial	Channelized
S2	Schwarzer Graben	Stream	52.56488	13.34918	0	0	50	50	Natural	Channelized
S3	Graben 1 Buch	Stream	52.62384	13.46883	0	100	0	0	Artificial	
S4	Graben 73 Buchholz	Stream	52.62881	13.45315	100	0	0	0	Artificial	
S5	Erpe	Stream	52.45888	13.61245	0	50	50	0	Natural	WWTP
S6	Koppelgraben	Stream	52.62065	13.41089	50	0	30	20	Unknown	
S7	Plumpengraben	Stream	52.41513	13.5628	0	0	100	0	Natural	Channelized

Table S2: Physico-chemical characteristics (mean ± SD and % variance explained) of four contrasting types of water bodies in the city of Berlin. Means and standard deviations were computed across all seasons and sites. The percentages of variance explained (% Var) refer to the effect of season within each water body type, calculated by type-II ANOVA (aka variance component analysis), with season treated as a random factor. F-values refer to results of repeated-measures ANOVAs testing for differences among water body types (* p<0.001, * p<0.05, ns = not significant).**

Water body	**Temperature**		**DOC**		**TP**		**NH_4^+**		**NO_3^-**		**Chlorophyll *a***	
type	**(°C)**	**% Var**	**(mg/L)**	**% Var**	**(mg/L)**	**% Var**	**(mg/L)**	**% Var**	**(mg/L)**	**% Var**	**(µg/L)**	**% Var**
Lakes	14.6 ± 6.9	94	7.5 ± 2.7	23	0.05 ± 0.05	34	0.07 ± 0.07	26	0.22 ± 0.36	48	6.2 ± 14.2	61
Ponds	13.7 ± 5.3	94	10.3 ± 3.0	32	0.09 ± 0.07	30	0.27 ± 0.67	30	0.03 ± 0.06	52	7.3 ± 7.7	55
Rivers	15.2 ± 6.2	92	8.0 ± 1.6	13	0.10 ± 0.08	43	0.15 ± 0.14	68	1.12 ± 1.66	46	2.1 ±2.9	51
Streams	11.3 ± 4.9	87	11.7 ± 5.5	42	0.26 ± 0.31	21	0.36 ± 0.65	76	0.91 ± 1.53	43	5.3 ± 9.7	53
$F_{water\ body}$	9.4***		3.8*		2.8^{ns}		1.3^{ns}		2.5^{ns}		1.0^{ns}	

Table S3: Description of absorbance and fluorescence indices.

Variable	Description
$SUVA_{254}$	Proxy for DOM aromaticity (Weishaar et al., 2003)
E2:E3	Ratio of absorbance at 250 and 365 nm, as an (inverse) indicator of molecular size (Peuravuori and Pihlaja, 1997) (Chen et al., 1977)
E4:E6	Indicator of humification (Chen et al., 1977)
SR	Ratio of slopes (SR) computed from short and long wavelength regions as another negative correlate with DOM molecular weight (Loiselle et al., 2009)
FI	Fluorescence index (FI) Ratio of the fluorescence intensities at the emissions 470 and 520 (obtained at excitation wavelength of 370nm). Indicator of DOM derived from terrestrial plants (FI around 1.2) or from microbes or algae (FI around 1.4) (Fellman et al., 2010; Cory and Mcknight, 2005; Cory et al., 2010; Jaffé et al., 2008)
HIX	Humification index (HIX) as a proxy for humic substances (Ohno, 2002)
β/α	Freshness index β/α (Wilson and Xenopoulos, 2009), which indicates the relative importance of recently produced DOM (Parlanti et al., 2000)

Table S4: Designation, excitation (Ex) and emission (Em) wavelengths of PARAFAC components, and the number of studies with matching components reported in OpenFluor (checked on the 28th March 2022) (Murphy et al., 2014).

PARAFAC component	Ex	Em	OpenFluor reference matches (0.95)	Explanation and selected references
C1	250	446	12	Humic-like, peak A (Coble, 1996); humic-like and recalcitrant (C1) (Hansen et al., 2016)
C2	250	500	70	Terrestial humic-like in waste water treatment impacted water, (G1) (Murphy et al., 2011); ubiquitous and recalcitrant humic (C2) (Chen et al., 2017)
C3	306	408	20	Humic-like, peak M (Coble, 1996); humic-like (C3) (Stedmon and Markager, 2005)
C4	256	444	8	Terrestrial humic-like, suggested as photo-refractory (Yamashita et al., 2010); (C2) terrestrial humic-like (C3) (Williams et al., 2010)
C5	250	382	12	Anthropogenic, microbial humic-like (C6) (Williams et al., 2016)
C6	294	352	33	Similar to tryptophan (C3) (Catalán et al., 2015); protein-like, linked to autochthonous production (C3) (Amaral et al., 2016)
C7	276	326	68	Protein-like, peak B (Coble, 1996); waste water treatment protein (C2) (Teymouri, 2007)

Table S5: Variables of absorbance and fluorescence analyses (mean ± SD and % variance explained) in contrasting types of urban surface waters. Means and standard deviations were computed across all seasons and sites. The percentages of variance explained (% Var) refer to the effect of season within each water body type, calculated by a type-II ANOVA (aka variance component analysis), with season treated as a random factor. F-values refer to results of repeated-measures ANOVA testing for differences among water body types (*p<0.001, **p<0.01, *p<0.05, ns = not significant). Abbreviations explained in Table B2**.

Water body type	**$SUVA_{254}$**		**E2:E3**		**E4:E6**		**SR**		**FI**		**HIX**		**β/α**	
		% Var		% Var		% Var		% Var		% Var		% Var		% Var
Lakes	1.55 ± 0.39	20	8.99 ± 2.14	6	3.02± 1.34	67	1.38 ± 0.27	12	1.61 ± 0.08	69	0.77 ± 0.08	9	0.86 ± 0.09	12
Ponds	2.14 ± 0.51	37	6.65 ± 1.24	14	3.12± 0.74	46	1.20 ± 0.19	29	1.52 ± 0.06	61	0.83 ± 0.04	47	0.70 ± 0.04	35
Rivers	2.25 ± 0.15	55	7.04 ± 0.98	12	4.40± 14.27	80	0.017 ± 0.002	76	1.68 ±0.11	10	0.85 ± 0.03	24	0.79 ± 0.09	19
Streams	2.50 ±0.52	65	6.328 ± 0.876	54	3.53± 2.31	75	0.97 ± 0.13	22	1.63 ± 0.14	11	0.86 ± 0.05	21	0.73 ± 0.10	24
$F_{water\ body}$	11.8***		5.8**		2.6 ns		9.2***		3.5*		4.9**		5.5**	

Table S6: PARAFAC components (mean ± SD and % variance explained) in contrasting types of urban surface waters. Means and standard deviations were computed across all seasons and sites. The percentages of variance explained (% Var) refer to the effect of season within each water body type, calculated by a type-II ANOVA (aka variance component analysis), with season treated as a random factor. F-values refer to results of repeated-measures ANOVA testing for differences among water body types (*p<0.001, **p<0.01, *p<0.05, ns = not significant).**

Water body type	**C1**		**C2**		**C3**		**C4**		**C5**		**C6**		**C7**	
		% Var		% Var		% Var		% Var		% Var		% Var		% Var
Lakes	0.17 ± 0.10	17	0.13 ± 0.06	14	0.24 ± 0.12	20	0.28 ± 0.12	14	0.31 ± 0.18	11	0.19 ± 0.10	15	0.18 ± 0.11	9
Ponds	0.24 ± 0.14	73	0.24 ± 0.11	80	0.40 ± 0.22	63	0.46 ± 0.21	63	0.52 ± 0.38	73	0.16 ± 0.11	65	0.25 ± 0.14	45
Rivers	0.51 ± 0.34	8	0.34 ± 0.17	12	0.66 ± 0.37	10	0.44 ± 0.12	32	0.61 ± 0.26	30	0.32 ± 0.22	14	0.25 ± 0.14	14
Streams	0.76 ± 0.47	16	0.57 ± 0.30	53	1.00 ± 0.58	30	0.85 ± 0.63	64	1.08 ± 0.73	16	0.37 ± 0.29	25	0.35 ± 0.18	45
Fwater body	6.3**		10.4***		7.6***		7.2***		8.4***		2.2n.s		2.6n.s.	

Table S7: Results of size exclusion chromatography (mean ± SD and % variance explained) of samples from contrasting types of urban surface waters. Means and standard deviations were computed across all seasons and sites. The percentages of variance explained (% Var) refer to the effect of season within each water body type, calculated by a type-II ANOVA (aka variance component analysis), with season treated as a random factor. F-values refer to results of repeated-measures ANOVA testing for differences among water body types (*p<0.001, **p<0.01, *p<0.05, ns = not significant). HS, humic-like substances; HMWS, high-molecular weight non-humic substances; and LMWS, low-molecular weight substances.**

Water body type	HMSW		HMSW		HS		HS		LMWS	
	(mg C/L)	% Var	(mg N/L)	% Var	(mg C/L)	% Var	(mg N/L)	% Var	(mg C/L)	% Var
Lakes	0.96 ± 0.74	27	0.11 ± 0.07	9	4.14 ± 1.49	19	0.25 ± 0.11	12	0.83 ± 0.26	18
Ponds	1.32 ± 0.60	41	0.16 ± 0.06	36	6.29 ± 2.42	26	0.33 ± 0.13	17	1.19 ± 0.46	45
Rivers	0.59 ± 0.20	60	0.09 ± 0.03	24	5.21 ± 0.97	33	0.31 ± 0.09	31	1.10 ± 0.41	22
Streams	0.73 ± 0.45	52	0.10 ± 0.05	41	7.21 ± 3.75	25	0.41 ± 0.27	9	1.48 ± 0.62	39
$\mathbf{F_{water\ body}}$	4.2*		2.9^{ns}		2.9^{ns}		$1.3^{ns.}$		3.7*	

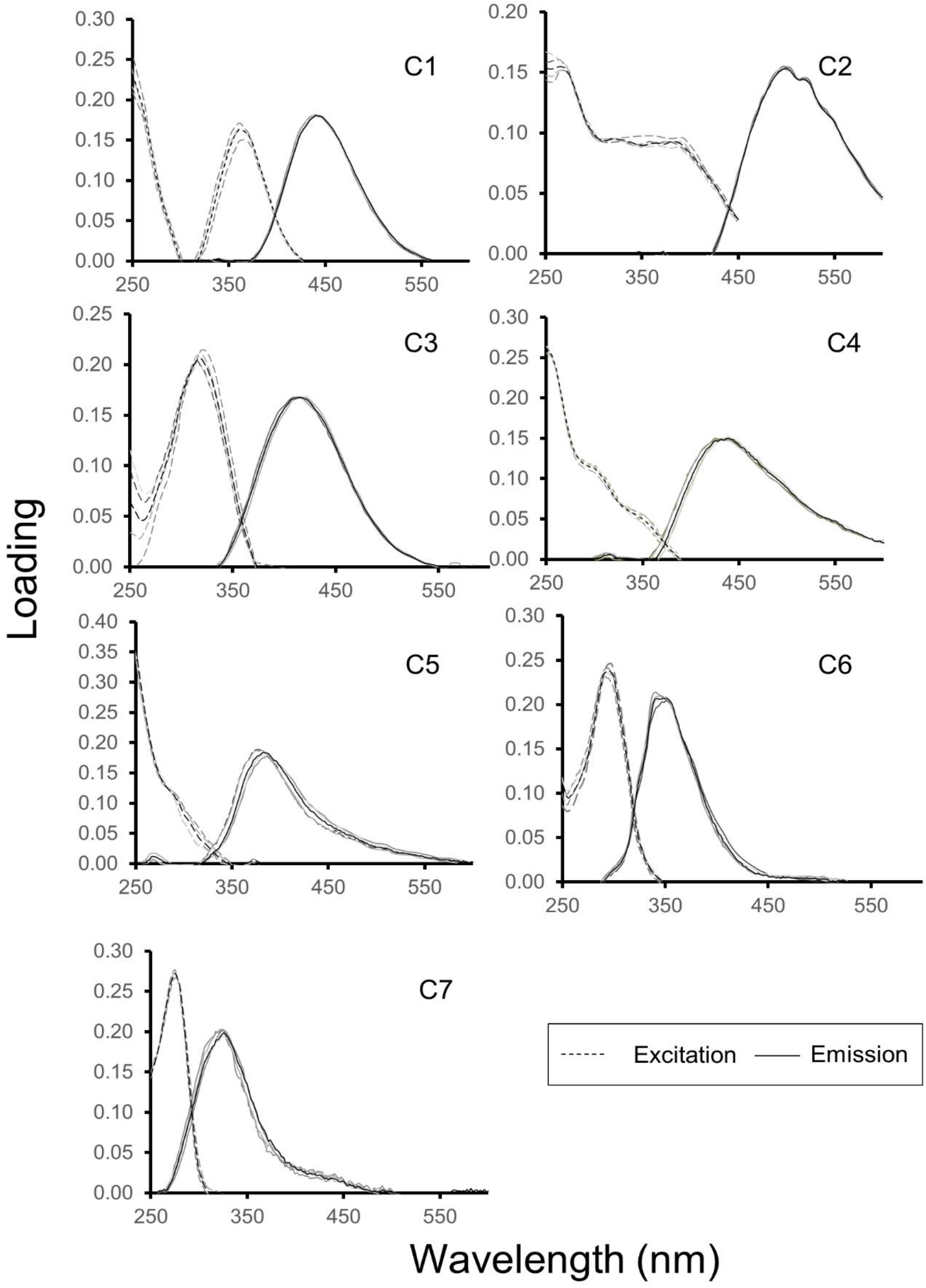

Figure S1 Emission and excitation wavelengths of PARAFAC components. Solid lines represent emission spectra, dashed lines excitation spectra. Lines in different shades of grey refer to models using different sample sub-sets of a split-half validation analysis.

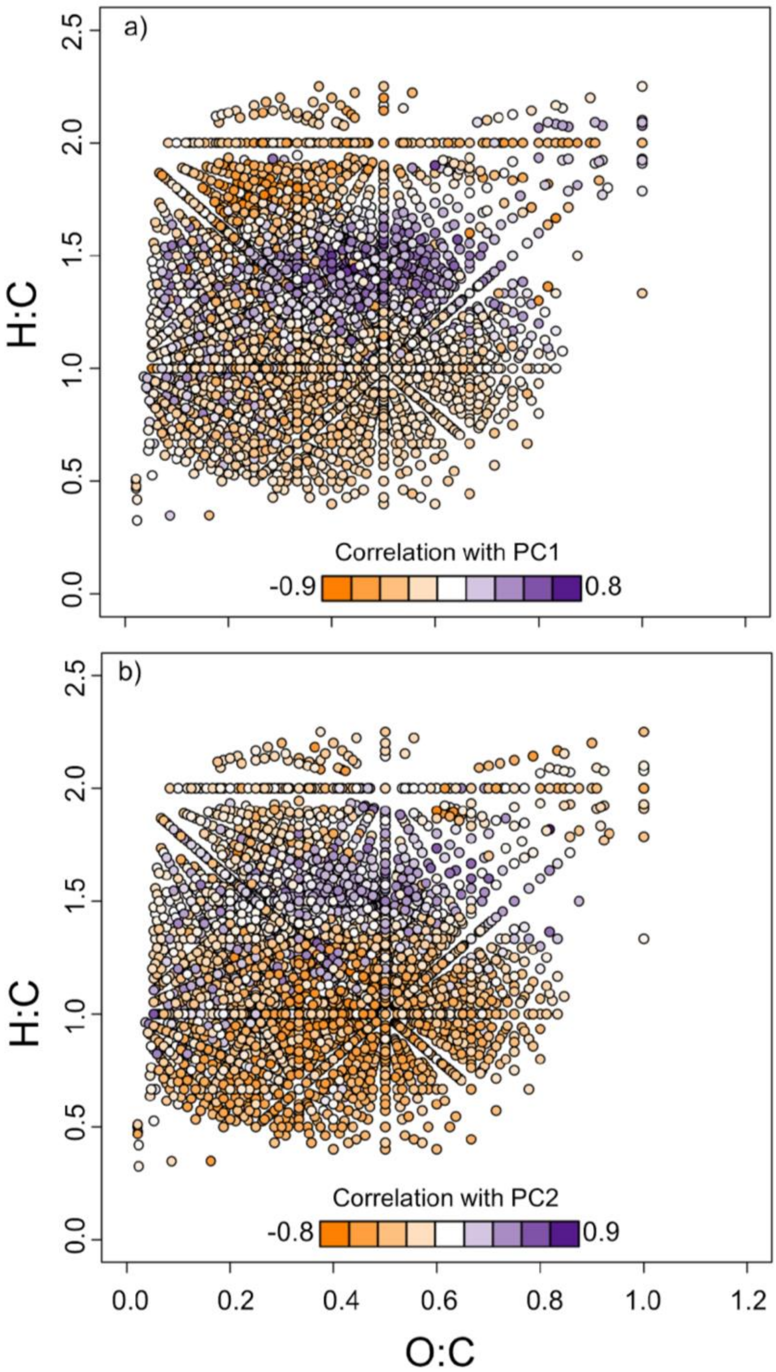

Figure S2 Van Krevelen plots showing all molecules (sum formulas) identified by FT-ICR-MS analysis of DOM samples collected at 32 urban sites over three seasons (summer, autumn and winter). Colour indicates molecule-specific Spearman correlation coefficients of the relative intensities of each compound with the first (a) and second (b) axis of the PCA shown in Figures 2 and 3. The data points were plotted in random order to avoid bias resulting from identical O:C and H:C ratios for many sum formulas.

Table S7: Trace organic compounds (TrOCs) analyzed in samples collected in urban surface waters. LLoQ = Limit of Quantification. Frequency refers to the number of occasions where concentrations exceeded the LLoQ.

Acronym	LLoQ (µg/L)	Frequency	Name	Description
ACS	0.1	72	Acesulfame	Sweetener
ATS	0.05	42	Amidrotrizoic	Radiocontrast agent
BTA	0.1	68	Benzotriazole	Corrosion inhibitor
BZF	0.1	6	Benzafibrate	Lipid-lowering agent
CBZ	0.05	44	Carbamazepine	Anticonvulsant
DCF	0.05	30	Diclofenac	Analgesic/anti-inflammatory agent
FAA	0.1	46	4-formylamin metabolite of metamizol	Analgesic
GAB	0.1	62	Gabapentin	Drug for epilepsy treatment/pain killer
GPL	0.05	39	Gabapentin-lactam	Derivate of gabapentin
IOM	0.1	40	Iomeprol	Radiocontrast agent
IOP	0.01	52	Iopromide	Radiocontrast agent
MBT	0.1	63	Methylbenzotriazole	Corrosion inhibitor
MTP	0.1	31	Metoprolol	Beta blocker
PRI	0.05	31	Primidone	Anticonvulsant
SMX	0.1	2	Sulfamethoxazole	Antibiotic
VAL	0.1	30	Valsartan	At1-receptor antagonist
VLX	0.1	3	Venlafaxine	Antidepressant
VSA	0.1	62	Valsartan acid	Antihypertensive agent

Table S8: Mean concentrations and standard deviations of Trace Organic Compound (TrOC) per water body type. See Table S7 for full names. BZF, SMX and VLX were always below the limit of quantification (LLoQ) and are hence omitted from the table.

	TrOC concentration (µg/L)			
Acronym	**Lakes**	**Ponds**	**Rivers**	**Streams**
ACS	0.23 ± 0.17	0.15 ± 0.16	0.28 ± 0.17	0.78 ± 1.35
ATS	0.08 ± 0.12	<LLoQ	0.74 ± 1.12	0.43 ± 0.88
BTA	0.34 ± 0.51	0.38 ± 0.91	2.37 ± 3.31	2.16 ± 3.61
CBZ	0.07 ± 0.08	<LLoQ	0.37 ± 0.48	0.41 ± 0.66
DCF	<LLoQ	<LLoQ	0.97 ± 1.38	0.88 ± 2.14
FAA	0.15 ± 0.23	<LLoQ	1.25 ± 1.66	2.10 ± 4.25
GAB	0.27 ± 0.36	<LLoQ	0.42 ± 0.43	0.74 ± 1.12
GPL	0.10 ± 0.17	<LLoQ	0.19 ± 0.42	0.13 ± 0.18
IOM	0.18 ± 0.28	<LLoQ	1.18 ± 2.36	1.44 ± 2.91
IOP	0.09 ± 0.19	0.01 ± 0.02	0.27 ± 0.32	1.46 ± 3.79
MBT	0.27 ± 0.39	0.11 ± 0.24	0.91 ± 1.01	0.69 ± 1.27
MTP	<LLoQ	<LLoQ	0.47 ± 0.58	0.63 ± 1.55
PRI	0.03 ± 0.02	<LLoQ	0.16 ± 0.22	0.26 ± 0.52
VAL	<LLoQ	<LLoQ	0.39 ± 0.44	0.97 ± 3.65
VSA	0.70 ± 1.02	<LLoQ	3.22 ± 3.84	3.33 ± 5.72

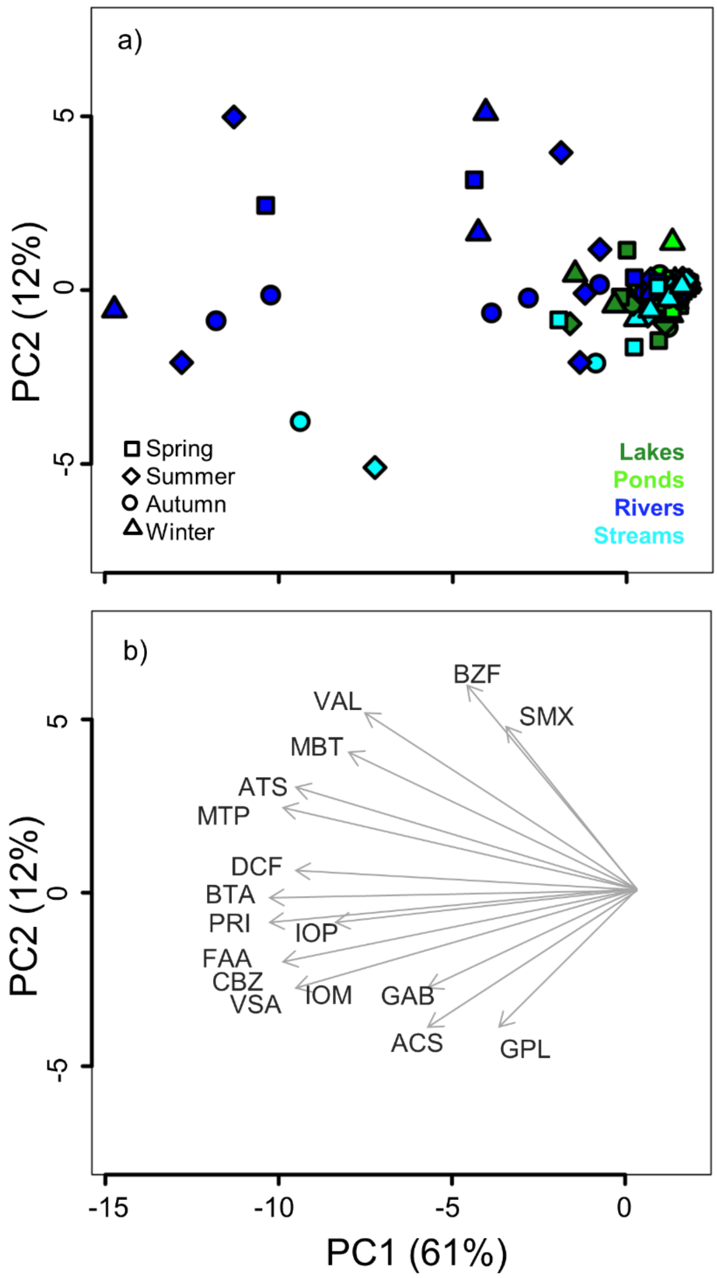

Figure S3 Principal Component Analysis (PCA) of 32 urban sites in the city of Berlin over four seasons (a) and Trace Organic Compounds (TrOCs) (b). Site S5 had extreme PC1 and PC2 scores; the site was included in the analysis but is not presented in the biplot to better visualize variability among the other sites. Abbreviations of the TrOCs (B) are explained in Table S7.

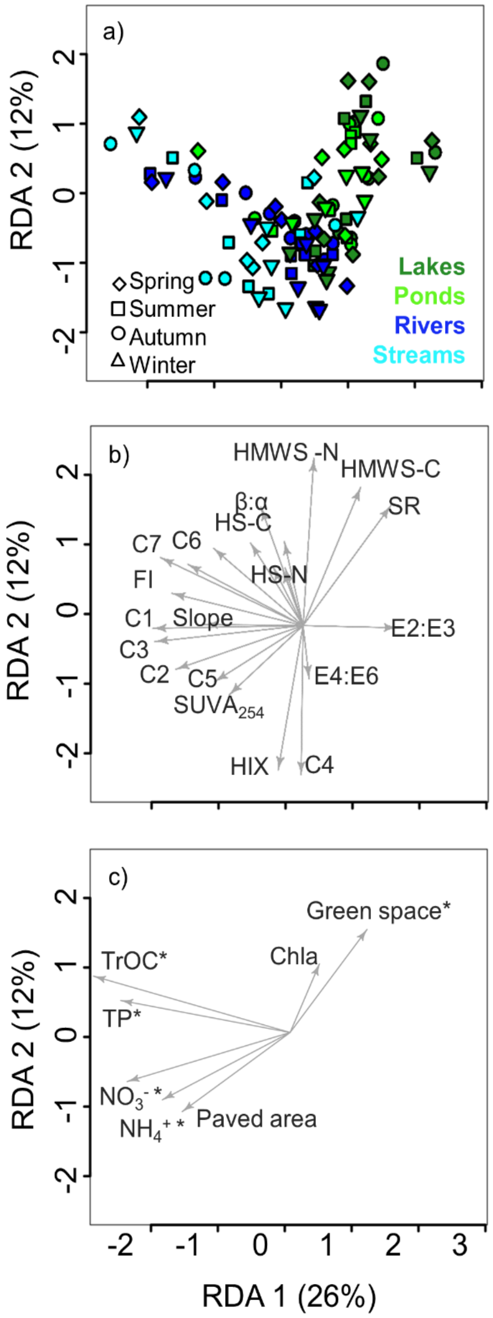

Figure S4 Redundancy Analysis (RDA) of urban sampling sites (a) visited 4 times over one year, the DOM characteristics included in the analysis (b) and the predictor variables (c), the last marked by an asterisk (*) when significant. DOM characteristics include (i) absorbance and fluorescence indexes (E2:E3, molecular size, E4:E6, indicator of humification, SR, slope ratio, β:α, freshness index, $SUVA_{254}$ and HIX, humification index), (ii) PARAFAC components (C1 to C7), and (iii) fractions derived from size exclusion chromatography (HS, humic-like substances; HMWS, high-molecular weight non-humic substances; and LMWS, low-molecular weight substances).

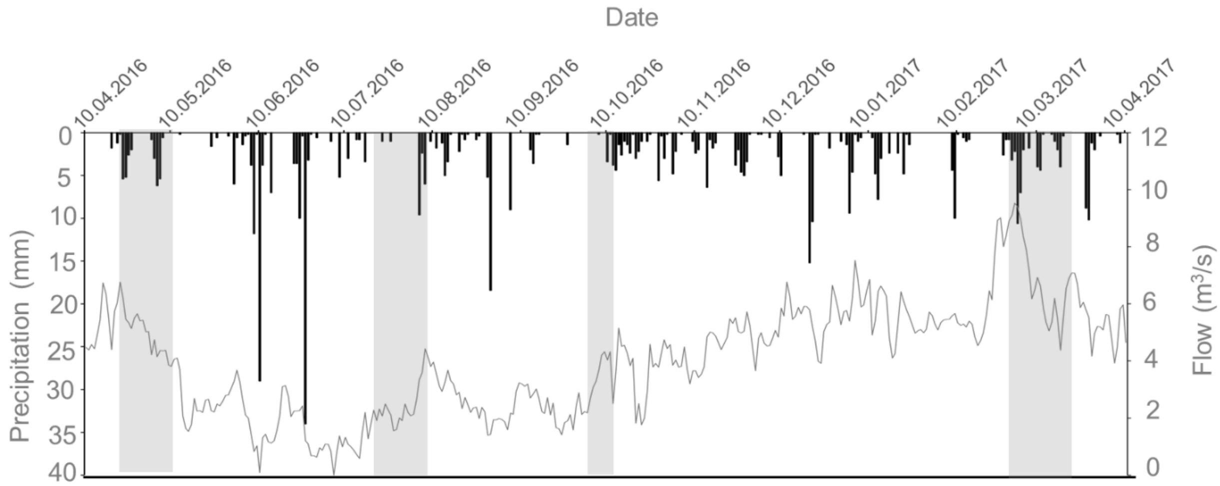

Figure S5 Precipitation and flow at a site within the city of Berlin during the study period, with the grey boxes indicating the four sampling periods.

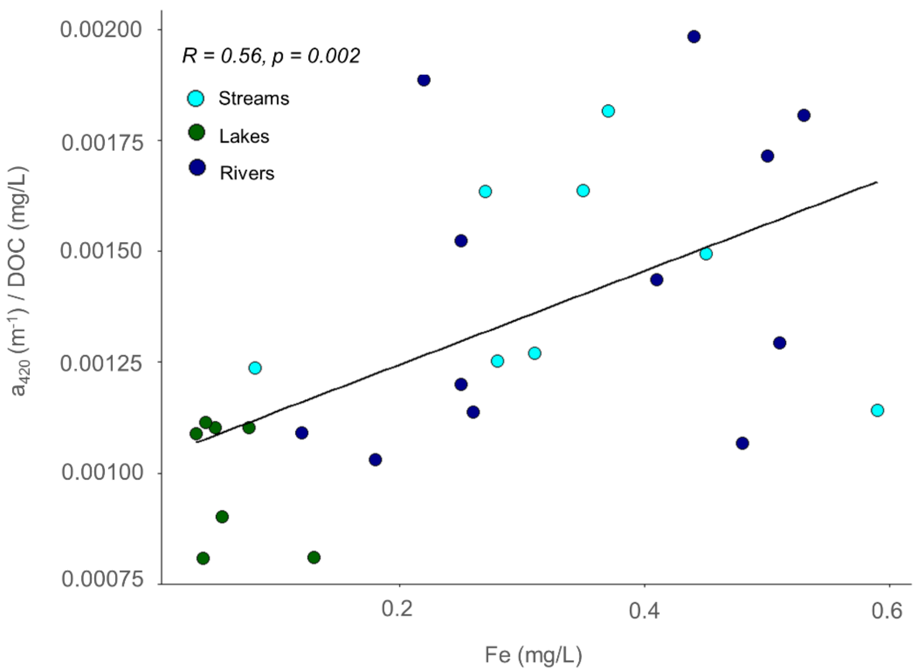

Figure S6 Relationship between iron (Fe) and the absorbance at 420nm relative to DOC(a420/DOC)

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