

Changes in optical properties and molecular composition of dissolved organic matter and formation of disinfection by-products during conventional water treatment processes

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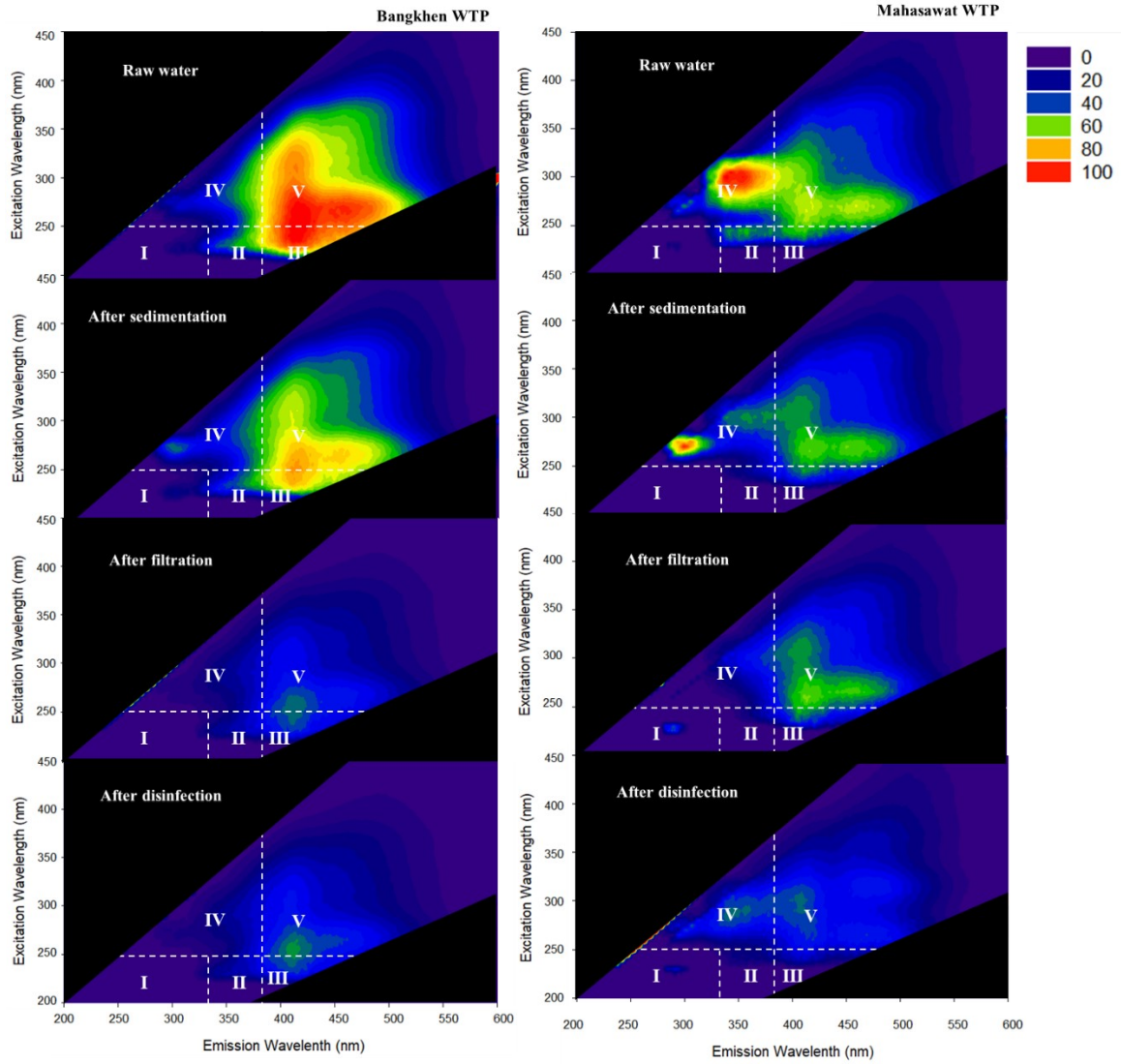


Figure S1 Excitation and emission spectra of BK-WTP and MH-WTP

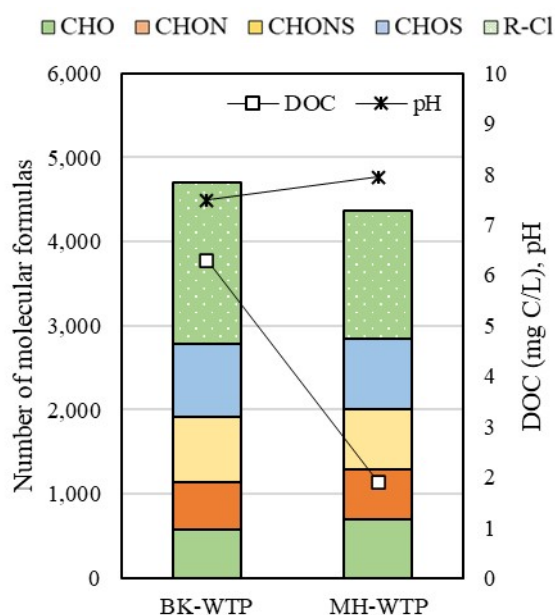


Figure S2 Number of molecular formulas of DOM in raw water samples of BK-WTP and MH-WTP

DOM components in raw water samples of BK-WTP and MH-WTP were classified according to heteroatoms assigned in the molecular formulas. The classification includes molecular formulas contain carbon, hydrogen and oxygen (CHO), CHO and nitrogen and sulfur heteroatoms (CHON, CHOS and CHONS) and molecular formulas containing chlorine (R-Cl). In total, 4701 and 4362 molecular formulas satisfied the assignment criteria for BK-WTP and MH-WTP (Figure S2), respectively. Collectively, the total absolute intensity of the molecular formulas accounted for 7.66×10^{10} and 3.27×10^{10} for BK-WTP and MH-WTP, respectively. This was quite consistent with DOC concentrations in the samples (6.3 mg/L for BK-WTP and 1.9 mg/L for MH-WTP).

DOM in RW of Both WTPs had similar portions of CHO, CHON, CHOS, CHONS and R-Cl. For BK-WTP, the portions were 12.3%, 12.0%, 18.5%, 16.4%, and 40.8% for CHO, CHON, CHOS, CHONS, and R-Cl, respectively. For MH-WTP, the portions were 16.0%, 13.5%, 19.1%, 16.5% and 34.9% for CHO, CHON, CHOS, CHONS and R-Cl, respectively. The largest portion of both WTPs was R-Cl and CHOS components. The presence of R-Cl in our samples were not surprising since the raw water samples were from the rivers which retrieve tremendously diverse DOM sources (wastewater effluent and agricultural runoff) along the lengths of the rivers. Moreover, R-Cl can naturally be produced from biological processes number of organisms ranging from bacteria, algae, lichens, plants and insects^{1,2}.

References

1. G. Öberg, The natural chlorine cycle—fitting the scattered pieces, *Applied microbiology and biotechnology*, 2002, **58**, 565-581.
2. G. W. Gribble, The diversity of naturally produced organohalogens, *Chemosphere*, 2003, **52**, 289-297.

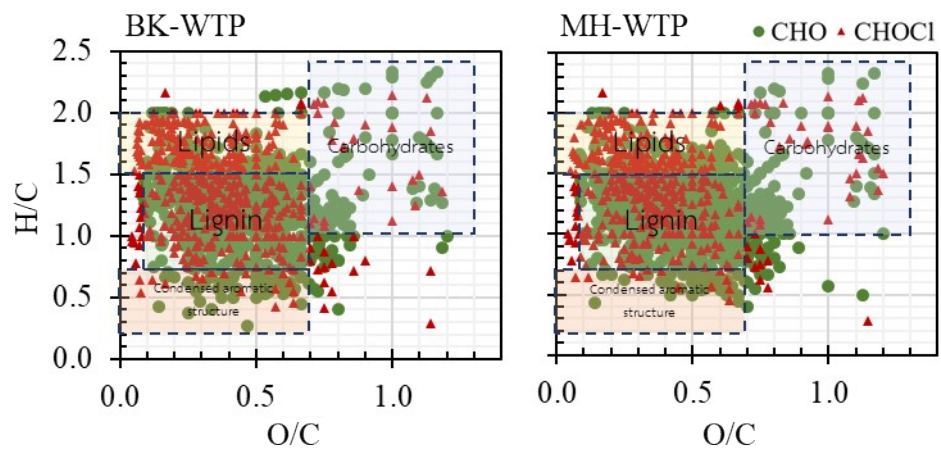


Figure S2-S3 van Krevelen diagrams of raw water samples of BK-WTP and MH-WTP

Table S1 Molecular characteristics of DOM components classified according to changes between two adjacent processes of BK-WTP

		BK-WTP					ANOVA <i>p</i> -value
		Disappeared	Decreased	Constant	Increased	Newly formed	
After sedimentation	Total number	191	469	295	78	99	-
	H/C	1.30	1.28	1.28	1.25	1.26	0.84
	O/C	0.45	0.45	0.42	0.45	0.51	<0.05
	DBE	5.70	5.59	5.82	5.46	5.81	0.86
	DBE-O	-0.38	-0.12	0.09	-0.26	-0.65	0.43
	AI	0.60	0.23	0.23	0.13	0.32	<0.05
	MW	327.07	294.15	304.87	291.57	298.87	<0.05
After filtration	Total number	121	113	393	314	160	-
	H/C	1.33	1.35	1.30	1.21	1.28	<0.05
	O/C	0.45	0.42	0.42	0.48	0.44	<0.05
	DBE	5.56	6.10	5.86	5.35	5.09	<0.05
	DBE-O	-0.63	-0.27	0.17	-0.23	-0.18	0.22
	AI	0.24	0.21	0.20	0.26	0.27	0.87
	MW	307.78	326.30	298.59	282.69	303.98	<0.05
After disinfection	Total number	49	59	763	109	65	-
	H/C	1.26	1.27	1.28	1.20	1.33	0.21
	O/C	0.44	0.48	0.44	0.48	0.47	0.29
	DBE	6.00	5.44	5.57	5.66	4.94	<0.05
	DBE-O	-0.08	-0.34	-0.07	0.09	-1.26	<0.05
	AI	0.25	0.10	0.23	0.30	0.39	0.54
	MW	313.85	286.52	299.20	284.83	325.60	<0.05

Table S2 Molecular characteristics of DOM components classified according to changes between two adjacent processes of MH-WTP

		MH-WTP					
		Disappeared	Decreased	Constant	Increased	Newly formed	ANOVA <i>p</i> -value
After sedimentation	Total number	118	279	527	173	66	-
	H/C	1.33	1.29	1.29	1.20	1.11	<0.05
	O/C	0.48	0.44	0.45	0.47	0.51	0.15
	DBE	6.93	6.64	5.77	4.80	5.11	<0.05
	DBE-O	-0.94	-0.17	-0.22	0.01	-0.08	0.23
	AI	0.56	0.21	0.28	0.25	0.19	<0.05
	MW	382.39	339.24	302.48	243.41	264.90	<0.05
After filtration	Total number	121	139	607	178	68	-
	H/C	1.19	1.27	1.27	1.27	1.38	<0.05
	O/C	0.52	0.46	0.44	0.45	0.42	<0.05
	DBE	6.62	5.83	5.69	5.60	5.53	<0.05
	DBE-O	-0.45	-0.31	-0.04	-0.26	-0.50	0.63
	AI	0.33	0.15	0.30	0.10	0.12	<0.05
	MW	325.49	301.10	298.04	289.32	328.55	<0.05
After disinfection	Total number	154	161	211	466	125	-
	H/C	1.40	1.43	1.29	1.18	1.07	<0.05
	O/C	0.40	0.38	0.42	0.49	0.53	<0.05
	DBE	5.36	4.78	6.15	5.89	6.37	<0.05
	DBE-O	-0.27	-0.37	0.15	-0.17	0.14	0.53
	AI	0.30	0.36	0.29	0.14	0.28	<0.05
	MW	318.59	317.51	314.52	279.10	295.19	<0.05

Table S3 List of DBPs detected in BK-WTP and MH-WTP

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
1	C ₂ H ₂ OCl ₂	111.9483	111.9485	2.05	MH-WTP	
2	C ₄ H ₃ O ₃ Cl	133.9771	133.9767	2.63	MH-WTP	
3	C ₃ H ₃ O ₃ Cl	147.9927	147.9924	2.39	MH-WTP	
4	C ₄ H ₄ O ₂ Cl ₂	153.9588	153.9583	3.74	MH-WTP	
5	C ₆ H ₅ O ₃ Cl	159.9927	159.9925	1.64	MH-WTP	
6	C ₃ H ₆ O ₂ Cl ₂	167.9745	167.9742	1.70	MH-WTP	
7	C ₃ H ₈ O ₂ Cl ₂	169.9901	169.9894	4.09	BK-WTP	
8	C ₈ H ₇ O ₂ Cl	170.0135	170.0138	1.78	BK-WTP	
9	C ₈ H ₉ O ₂ Cl	172.0291	172.0288	1.85	MH-WTP	
10	C ₇ H ₇ O ₃ Cl	174.0084	174.0084	0.33	BK-WTP	
11	C ₆ H ₂ O ₂ Cl ₂	175.9432	175.9440	4.46	MH-WTP	
12	C ₆ H ₈ O ₂ Cl ₂	181.9901	181.9896	3.17	Both WTPs	
13	C ₃ H ₆ O ₃ Cl ₂	183.9694	183.9685	4.79	BK-WTP	
14	C ₄ H ₃ O ₄ Cl	185.9720	185.9715	2.79	Both WTPs	
15	C ₉ H ₁₁ O ₂ Cl	186.0448	186.0453	2.91	MH-WTP	
16	C ₄ H ₃ O ₂ Cl ₃	187.9199	187.9203	2.27	MH-WTP	
17	C ₈ H ₉ O ₃ Cl	188.0240	188.0243	1.58	MH-WTP	
18	C ₇ H ₇ O ₄ Cl	190.0033	190.0026	3.88	MH-WTP	
19	C ₃ H ₆ O ₄ Cl ₂	199.9643	199.9633	4.98	MH-WTP	
20	C ₁₁ H ₃ O ₂ Cl	201.9822	201.9816	2.56	MH-WTP	
21	C ₈ H ₆ O ₂ Cl ₂	203.9745	203.9754	4.48	MH-WTP	
22	C ₈ H ₉ O ₄ Cl	204.0189	204.0189	0.01	MH-WTP	
23	C ₈ H ₈ O ₂ Cl ₂	205.9901	205.9893	3.91	MH-WTP	
24	C ₇ H ₁₁ O ₅ Cl	210.0295	210.0291	2.06	MH-WTP	
25	C ₁₁ H ₁₁ O ₂ Cl	210.0448	210.0447	0.51	MH-WTP	
26	C ₉ H ₅ O ₄ Cl	211.9876	211.9867	4.47	Both WTPs	
27	C ₉ H ₇ O ₄ Cl	214.0033	214.0024	4.15	MH-WTP	Gonsior et al. (2014)
28	C ₈ H ₅ O ₅ Cl	215.9826	215.9817	4.09	MH-WTP	Lavonen et al. (2013), Gonsior et al. (2014), Zhang et al. (2014)
29	C ₉ H ₉ O ₄ Cl	216.0189	216.0183	2.77	MH-WTP	Lavonen et al. (2013), Gonsior et al. (2014)
30	C ₁₀ H ₁₃ O ₃ Cl	216.0553	216.0547	2.70	MH-WTP	
31	C ₇ H ₄ O ₄ Cl ₂	221.9487	221.9478	3.99	MH-WTP	Gonsior et al. (2014), Zhang et al. (2014)
32	C ₁₃ H ₁₅ OCl	222.0811	222.0807	1.95	BK-WTP	Zhang et al. (2014)
33	C ₁₀ H ₅ O ₄ Cl	223.9876	223.9867	4.23	MH-WTP	Gonsior et al. (2014), Zhang et al. (2014)
34	C ₈ H ₉ OCl ₃	225.9719	225.9717	0.70	BK-WTP	Zhang et al. (2014)
35	C ₁₁ H ₁₁ O ₃ Cl	226.0397	226.0391	2.40	MH-WTP	Zhang et al. (2014)
36	C ₆ H ₆ O ₅ Cl ₂	227.9592	227.9583	4.00	MH-WTP	Zhang et al. (2014)
37	C ₇ H ₁₀ O ₄ Cl ₂	227.9956	227.9948	3.62	MH-WTP	Zhang et al. (2014)
38	C ₁₀ H ₉ O ₄ Cl	228.0189	228.0181	3.50	MH-WTP	Gonsior et al. (2014), Zhang et al. (2014)

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
39	C ₁₀ H ₁₁ O ₄ Cl	230.0346	230.0337	3.99	MH-WTP	Zhang et al. (2014)
40	C ₃ H ₃ O ₄ Cl ₃	231.9097	231.9089	3.42	MH-WTP	Zhang et al. (2014)
41	C ₈ H ₅ O ₆ Cl	231.9775	231.9764	4.52	Both WTPs	Zhang et al. (2014)
42	C ₁₀ H ₁₃ O ₄ Cl	232.0502	232.0495	3.05	MH-WTP	
43	C ₃ H ₃ O ₄ Cl ₃	233.9253	233.9251	1.21	MH-WTP	
44	C ₆ H ₉ O ₃ Cl ₃	233.9617	233.9610	3.20	MH-WTP	
45	C ₈ H ₇ O ₆ Cl	233.9931	233.9924	3.11	MH-WTP	Gonsior et al. (2014)
46	C ₉ H ₁₁ O ₅ Cl	234.0295	234.0288	2.96	MH-WTP	
47	C ₁₀ H ₁₅ O ₄ Cl	234.0659	234.0659	0.18	BK-WTP	
48	C ₈ H ₉ O ₆ Cl	236.0088	236.0079	3.85	MH-WTP	
49	C ₈ H ₈ O ₄ Cl ₂	237.9800	237.9793	2.71	Both WTPs	
50	C ₇ H ₈ O ₅ Cl ₂	241.9749	241.9740	3.76	MH-WTP	
51	C ₁₂ H ₁₂ OCl ₂	242.0265	242.0255	4.38	BK-WTP	
52	C ₇ H ₁₀ O ₅ Cl ₂	243.9905	243.9898	3.16	BK-WTP	
53	C ₁₁ H ₁₃ O ₄ Cl	244.0502	244.0492	4.17	MH-WTP	Lavonen et al. (2013)
54	C ₁₀ H ₁₁ O ₅ Cl	246.0295	246.0287	3.39	MH-WTP	Lavonen et al. (2013)
55	C ₇ H ₁₅ O ₇ Cl	246.0506	246.0509	0.88	MH-WTP	
56	C ₁₁ H ₁₅ O ₄ Cl	246.0659	246.0652	2.71	MH-WTP	Lavonen et al. (2013)
57	C ₉ H ₉ O ₆ Cl	248.0088	248.0080	3.06	Both WTPs	Lavonen et al. (2013)
58	C ₁₁ H ₁₇ O ₄ Cl	248.0815	248.0812	1.32	BK-WTP	
59	C ₈ H ₄ O ₅ Cl ₂	249.9436	249.9448	4.88	MH-WTP	Zhang et al. (2014)
60	C ₉ H ₁₁ O ₆ Cl	250.0244	250.0238	2.31	MH-WTP	Zhang et al. (2014)
61	C ₁₀ H ₁₅ O ₅ Cl	250.0608	250.0601	2.73	MH-WTP	Zhang et al. (2014)
62	C ₈ H ₆ O ₅ Cl ₂	251.9592	251.9582	4.25	Both WTPs	Zhang et al. (2014)
63	C ₇ H ₅ O ₈ Cl	251.9673	251.9673	0.17	BK-WTP	Zhang et al. (2014)
64	C ₉ H ₁₀ O ₄ Cl ₂	251.9956	251.9946	4.03	MH-WTP	Zhang et al. (2014)
65	C ₈ H ₈ O ₅ Cl ₂	253.9749	253.9744	2.09	MH-WTP	Zhang et al. (2014)
66	C ₁₄ H ₃ O ₃ Cl	253.9771	253.9772	0.58	MH-WTP	Zhang et al. (2014)
67	C ₈ H ₁₁ O ₇ Cl	254.0193	254.0186	2.73	MH-WTP	Zhang et al. (2014)
68	C ₁₂ H ₁₁ O ₄ Cl	254.0346	254.0337	3.42	MH-WTP	Zhang et al. (2014)
69	C ₁₂ H ₁₃ O ₄ Cl	256.0502	256.0496	2.37	MH-WTP	Zhang et al. (2014)
70	C ₁₀ H ₇ O ₆ Cl	257.9931	257.9926	2.20	MH-WTP	Lavonen et al. (2013)
71	C ₁₁ H ₁₁ O ₅ Cl	258.0295	258.0287	3.00	MH-WTP	Lavonen et al. (2013)
72	C ₁₆ H ₁₅ OCl	258.0811	258.0822	4.17	BK-WTP	
73	C ₆ H ₃ O ₅ Cl ₃	259.9046	259.9038	3.19	Both WTPs	
74	C ₁₀ H ₆ O ₄ Cl ₂	259.9643	259.9635	3.22	MH-WTP	Zhang et al. (2014)
75	C ₁₀ H ₉ O ₆ Cl	260.0088	260.0081	2.49	MH-WTP	Zhang et al. (2014)
76	C ₁₁ H ₁₃ O ₅ Cl	260.0452	260.0445	2.47	MH-WTP	Zhang et al. (2014)
77	C ₁₀ H ₁₉ OCl ₃	260.0501	260.0490	4.53	BK-WTP	Zhang et al. (2014)
78	C ₉ H ₇ O ₇ Cl	261.9880	261.9876	1.77	MH-WTP	Zhang et al. (2014)

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
79	C ₁₁ H ₁₅ O ₅ Cl	262.0608	262.0603	1.96	MH-WTP	Zhang et al. (2014)
80	C ₆ H ₇ O ₅ Cl ₃	263.9359	263.9352	2.61	MH-WTP	Zhang et al. (2014)
81	C ₁₄ H ₁₃ O ₃ Cl	264.0553	264.0551	0.73	MH-WTP	Zhang et al. (2014)
82	C ₁₁ H ₁₇ O ₅ Cl	264.0765	264.0760	1.64	MH-WTP	Zhang et al. (2014)
83	C ₉ H ₈ O ₅ Cl ₂	265.9749	265.9741	2.90	Both WTPs	Zhang et al. (2014)
84	C ₉ H ₆ O ₆ Cl ₂	267.9541	267.9532	3.42	Both WTPs	Zhang et al. (2014)
85	C ₈ H ₉ O ₈ Cl	267.9986	267.9987	0.34	BK-WTP	
86	C ₉ H ₁₃ O ₇ Cl	268.0350	268.0341	3.22	MH-WTP	
87	C ₁₆ H ₂₇ OCl	270.1750	270.1750	0.31	BK-WTP	
88	C ₁₂ H ₁₃ O ₅ Cl	272.0452	272.0444	2.69	MH-WTP	Lavonen et al. (2013)
89	C ₁₄ H ₂₁ O ₅ Cl	272.1179	272.1175	1.52	BK-WTP	
90	C ₁₁ H ₈ O ₄ Cl ₂	273.9800	273.9789	3.82	BK-WTP	Lavonen et al. (2013), Zhang et al. (2014)
91	C ₁₁ H ₁₁ O ₆ Cl	274.0244	274.0240	1.60	MH-WTP	Lavonen et al. (2013)
92	C ₁₂ H ₁₅ O ₅ Cl	274.0608	274.0600	2.93	MH-WTP	Lavonen et al. (2013)
93	C ₁₁ H ₂₁ OCl ₃	274.0658	274.0647	3.90	BK-WTP	
94	C ₁₀ H ₉ O ₇ Cl	276.0037	276.0030	2.58	MH-WTP	Lavonen et al. (2013), Phungsai et al. (2018)
95	C ₁₁ H ₁₃ O ₆ Cl	276.0401	276.0394	2.31	MH-WTP	Lavonen et al. (2013), Phungsai et al. (2018)
96	C ₁₀ H ₁₉ O ₂ Cl ₃	276.0451	276.0440	3.82	BK-WTP	
97	C ₁₃ H ₁₃ O ₅ Cl	276.0553	276.0551	0.99	MH-WTP	
98	C ₁₂ H ₁₇ O ₅ Cl	276.0765	276.0759	2.08	MH-WTP	Lavonen et al. (2013)
99	C ₁₀ H ₁₁ O ₇ Cl	278.0193	278.0186	2.49	Both WTPs	Lavonen et al. (2013), Phungsai et al. (2018)
100	C ₁₀ H ₁₃ O ₇ Cl	280.0350	280.0345	1.72	MH-WTP	
101	C ₁₄ H ₁₃ O ₄ Cl	280.0502	280.0491	4.10	Both WTPs	Lavonen et al. (2013)
102	C ₁₁ H ₁₇ O ₆ Cl	280.0714	280.0707	2.39	MH-WTP	Lavonen et al. (2013)
103	C ₁₇ H ₁₁ O ₂ Cl	282.0448	282.0442	1.84	Both WTPs	
104	C ₁₁ H ₁₉ O ₆ Cl	282.0870	282.0864	2.37	MH-WTP	
105	C ₁₁ H ₅ O ₇ Cl	283.9724	283.9712	4.24	MH-WTP	
106	C ₁₂ H ₉ O ₆ Cl	284.0088	284.0075	4.43	MH-WTP	Lavonen et al. (2013)
107	C ₁₁ H ₁₅ O ₂ Cl ₃	284.0138	284.0126	4.24	BK-WTP	
108	C ₁₃ H ₁₃ O ₅ Cl	284.0452	284.0444	2.79	MH-WTP	Lavonen et al. (2013)
109	C ₈ H ₅ O ₅ Cl ₃	285.9203	285.9192	3.60	MH-WTP	
110	C ₉ H ₁₂ O ₆ Cl ₂	286.0011	286.0004	2.57	MH-WTP	Zhang et al. (2014)
111	C ₁₂ H ₁₁ O ₆ Cl	286.0244	286.0233	3.77	MH-WTP	Zhang et al. (2014)
112	C ₁₃ H ₁₅ O ₅ Cl	286.0608	286.0600	2.88	MH-WTP	Zhang et al. (2014)
113	C ₁₀ H ₁₅ O ₃ Cl ₃	288.0087	288.0075	4.23	BK-WTP	Zhang et al. (2014)
114	C ₁₂ H ₁₃ O ₆ Cl	288.0401	288.0392	2.87	MH-WTP	Zhang et al. (2014)
115	C ₉ H ₁₇ O ₈ Cl	288.0612	288.0612	0.10	MH-WTP	Zhang et al. (2014)
116	C ₁₃ H ₁₇ O ₅ Cl	288.0765	288.0759	2.02	BK-WTP	Zhang et al. (2014)
117	C ₁₀ HO ₄ Cl ₃	289.8940	289.8927	4.64	MH-WTP	Zhang et al. (2014)
118	C ₇ H ₅ O ₆ Cl ₃	289.9152	289.9143	3.08	MH-WTP	Zhang et al. (2014)

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
119	C ₁₁ H ₁₁ O ₇ Cl	290.0193	290.0185	2.73	MH-WTP	Zhang et al. (2014), Phungsai et al. (2018)
120	C ₁₂ H ₁₅ O ₆ Cl	290.0557	290.0551	2.30	MH-WTP	Zhang et al. (2014)
121	C ₁₃ H ₂₇ O ₃ Cl	290.1649	290.1663	4.75	MH-WTP	
122	C ₁₁ H ₁₃ O ₇ Cl	292.0350	292.0343	2.34	MH-WTP	Lavonen et al. (2013)
123	C ₈ H ₁₇ O ₉ Cl	292.0561	292.0573	4.20	MH-WTP	
124	C ₁₂ H ₁₇ O ₆ Cl	292.0714	292.0707	2.39	Both WTPs	Lavonen et al. (2013)
125	C ₁₆ H ₁₇ O ₃ Cl	292.0866	292.0869	1.09	MH-WTP	
126	C ₁₀ H ₈ O ₆ Cl ₂	293.9698	293.9690	2.81	Both WTPs	Lavonen et al. (2013), Zhang et al. (2014)
127	C ₁₀ H ₁₁ O ₈ Cl	294.0142	294.0137	1.97	MH-WTP	
128	C ₁₇ H ₂₃ O ₃ Cl	294.1387	294.1376	3.49	BK-WTP	
129	C ₁₀ H ₁₂ O ₆ Cl ₂	298.0011	298.0003	2.77	BK-WTP	Lavonen et al. (2013), Zhang et al. (2014)
130	C ₁₃ H ₁₁ O ₆ Cl	298.0244	298.0231	4.29	MH-WTP	Lavonen et al. (2013)
131	C ₁₀ H ₁₄ O ₆ Cl ₂	300.0167	300.0155	4.22	MH-WTP	Zhang et al. (2014)
132	C ₁₂ H ₁₁ O ₇ Cl	302.0193	302.0184	3.19	Both WTPs	Zhang et al. (2014)
133	C ₁₂ H ₁₃ O ₇ Cl	304.0350	304.0343	2.35	MH-WTP	Zhang et al. (2014)
134	C ₁₃ H ₁₇ O ₆ Cl	304.0714	304.0706	2.66	MH-WTP	Zhang et al. (2014)
135	C ₁₁ H ₂₂ O ₃ Cl ₂	304.0844	304.0833	3.82	BK-WTP	Zhang et al. (2014)
136	C ₁₄ H ₂₁ O ₅ Cl	304.1078	304.1070	2.38	MH-WTP	Zhang et al. (2014)
137	C ₁₁ H ₈ O ₆ Cl ₂	305.9698	305.9687	3.58	MH-WTP	Zhang et al. (2014)
138	C ₁₁ H ₁₁ O ₈ Cl	306.0142	306.0137	1.73	MH-WTP	Zhang et al. (2014)
139	C ₉ H ₁₆ O ₇ Cl ₂	306.0273	306.0288	5.00	BK-WTP	Zhang et al. (2014)
140	C ₁₂ H ₁₇ O ₇ Cl	308.0663	308.0653	3.35	MH-WTP	Zhang et al. (2014)
141	C ₁₀ H ₈ O ₇ Cl ₂	309.9647	309.9637	3.29	MH-WTP	Zhang et al. (2014)
142	C ₁₈ H ₁₁ O ₃ Cl	310.0397	310.0412	4.93	BK-WTP	
143	C ₁₇ H ₂₃ O ₃ Cl	310.1336	310.1333	0.78	BK-WTP	
144	C ₁₃ H ₂₂ O ₄ Cl ₂	312.0895	312.0888	2.39	BK-WTP	
145	C ₁₀ H ₁₂ O ₇ Cl ₂	313.9960	313.9967	2.10	MH-WTP	Zhang et al. (2014)
146	C ₁₃ H ₂₁ O ₂ Cl ₃	314.0607	314.0600	2.40	BK-WTP	Zhang et al. (2014)
147	C ₁₀ H ₁₁ O ₅ Cl ₃	315.9672	315.9663	2.91	MH-WTP	Zhang et al. (2014)
148	C ₁₀ H ₁₄ O ₇ Cl ₂	316.0117	316.0107	3.07	MH-WTP	Zhang et al. (2014)
149	C ₁₃ H ₁₃ O ₇ Cl	316.0350	316.0341	2.95	MH-WTP	Zhang et al. (2014)
150	C ₁₄ H ₁₇ O ₆ Cl	316.0714	316.0708	1.67	MH-WTP	Zhang et al. (2014)
151	C ₁₁ H ₄ O ₇ Cl ₂	317.9334	317.9324	3.05	MH-WTP	Zhang et al. (2014)
152	C ₁₂ H ₁₁ O ₈ Cl	318.0142	318.0136	2.01	MH-WTP	Zhang et al. (2014)
153	C ₉ H ₁₅ O ₁₀ Cl	318.0354	318.0366	3.84	BK-WTP	Zhang et al. (2014)
154	C ₁₃ H ₁₅ O ₇ Cl	318.0506	318.0496	3.15	MH-WTP	Zhang et al. (2014), Phungsai et al. (2018)
155	C ₁₄ H ₁₉ O ₆ Cl	318.0870	318.0860	3.11	MH-WTP	Zhang et al. (2014)
156	C ₁₃ H ₂₃ O ₃ Cl	318.1234	318.1228	2.02	BK-WTP	Lavonen et al. (2013)
157	C ₈ H ₇ O ₇ Cl ₃	319.9257	319.9245	3.78	MH-WTP	
158	C ₁₁ H ₆ O ₇ Cl ₂	319.9491	319.9479	3.50	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
159	C ₁₂ H ₁₃ O ₈ Cl	320.0299	320.0304	1.41	MH-WTP	Lavonen et al. (2013), Phungsai et al. (2018)
160	C ₁₁ H ₁₉ O ₄ Cl ₃	320.0349	320.0342	2.26	BK-WTP	
161	C ₁₂ H ₂₃ O ₃ Cl ₃	320.0713	320.0704	2.72	BK-WTP	
162	C ₁₀ H ₄ O ₈ Cl ₂	321.9283	321.9272	3.37	BK-WTP	
163	C ₁₁ H ₈ O ₇ Cl ₂	321.9647	321.9633	4.51	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)
164	C ₁₂ H ₁₅ O ₈ Cl	322.0455	322.0456	0.01	MH-WTP	Lavonen et al. (2013)
165	C ₁₂ H ₁₇ O ₈ Cl	324.0612	324.0603	2.83	MH-WTP	Lavonen et al. (2013)
166	C ₁₀ H ₈ O ₈ Cl ₂	325.9596	325.9596	0.05	Both WTPs	
167	C ₁₂ H ₅ O ₉ Cl	327.9622	327.9614	2.45	MH-WTP	Lavonen et al. (2013)
168	C ₁₃ H ₁₇ O ₆ Cl	328.0714	328.0706	2.43	MH-WTP	Lavonen et al. (2013)
169	C ₁₆ H ₂₁ O ₅ Cl	328.1078	328.1071	1.90	BK-WTP	Lavonen et al. (2013)
170	C ₁₁ H ₁₉ O ₉ Cl	330.0718	330.0731	4.02	BK-WTP	
171	C ₁₃ H ₁₉ O ₆ Cl	330.0870	330.0861	2.66	MH-WTP	Lavonen et al. (2013)
172	C ₁₂ H ₉ O ₉ Cl	331.9935	331.9922	3.86	BK-WTP	Lavonen et al. (2013)
173	C ₁₄ H ₁₇ O ₇ Cl	332.0663	332.0656	2.15	MH-WTP	Lavonen et al. (2013)
174	C ₁₉ H ₁₈ OCl ₂	332.0735	332.0736	0.39	BK-WTP	
175	C ₁₅ H ₂₁ O ₆ Cl	332.1027	332.1016	3.10	MH-WTP	Lavonen et al. (2013)
176	C ₁₄ H ₂₇ O ₂ Cl ₃	332.1077	332.1069	2.30	BK-WTP	
177	C ₁₂ H ₂₅ O ₈ Cl	332.1238	332.1252	4.19	MH-WTP	
178	C ₈ H ₅ O ₈ Cl ₃	333.9050	333.9036	4.08	BK-WTP	
179	C ₁₂ H ₅ O ₅ Cl ₃	333.9203	333.9219	4.97	MH-WTP	
180	C ₁₀ H ₁₉ O ₁₀ Cl	334.0667	334.0680	3.90	BK-WTP	
181	C ₁₅ H ₂₀ O ₄ Cl ₂	334.0739	334.0728	3.13	BK-WTP	
182	C ₁₂ H ₁₀ O ₇ Cl ₂	335.9804	335.9791	3.66	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)
183	C ₁₂ H ₁₃ O ₉ Cl	336.0248	336.0245	0.96	MH-WTP	Lavonen et al. (2013)
184	C ₁₄ H ₂₁ O ₇ Cl	336.0976	336.0971	1.41	Both WTPs	Lavonen et al. (2013)
185	C ₁₁ H ₈ O ₈ Cl ₂	337.9596	337.9585	3.33	MH-WTP	Zhang et al. (2014)
186	C ₁₄ H ₂₃ O ₇ Cl	338.1132	338.1120	3.65	Both WTPs	Zhang et al. (2014)
187	C ₁₁ H ₁₀ O ₈ Cl ₂	339.9753	339.9739	4.05	Both WTPs	Zhang et al. (2014)
188	C ₁₂ H ₁₄ O ₇ Cl ₂	340.0117	340.0105	3.30	Both WTPs	Zhang et al. (2014)
189	C ₁₁ H ₁₃ O ₁₀ Cl	340.0197	340.0206	2.65	MH-WTP	Zhang et al. (2014)
190	C ₁₀ H ₈ O ₉ Cl ₂	341.9545	341.9536	2.78	MH-WTP	Zhang et al. (2014)
191	C ₁₆ H ₁₉ O ₆ Cl	342.0870	342.0866	1.34	Both WTPs	Zhang et al. (2014)
192	C ₁₄ H ₂₃ O ₃ Cl ₃	344.0713	344.0707	1.65	BK-WTP	Zhang et al. (2014)
193	C ₁₄ H ₁₅ O ₈ Cl	346.0455	346.0448	2.19	MH-WTP	Zhang et al. (2014)
194	C ₁₈ H ₁₅ O ₅ Cl	346.0608	346.0624	4.61	MH-WTP	Zhang et al. (2014)
195	C ₁₃ H ₁₉ O ₇ Cl	346.0819	346.0810	2.72	MH-WTP	Zhang et al. (2014)
196	C ₁₆ H ₂₃ O ₆ Cl	346.1183	346.1176	2.07	MH-WTP	Lavonen et al. (2013)
197	C ₁₅ H ₁₅ O ₃ Cl ₃	348.0087	348.0104	4.95	MH-WTP	
198	C ₁₆ H ₂₇ O ₆ Cl	350.1496	350.1490	1.79	MH-WTP	Lavonen et al. (2013)

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
199	C ₁₂ H ₁₀ O ₈ Cl ₂	351.9753	351.9739	3.82	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)
200	C ₁₃ H ₁₄ O ₇ Cl ₂	352.0117	352.0111	1.51	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)
201	C ₁₂ H ₂₃ O ₅ Cl ₃	352.0611	352.0604	2.16	BK-WTP	
202	C ₁₁ H ₅ O ₇ Cl ₃	353.9101	353.9089	3.30	MH-WTP	
203	C ₁₄ H ₂₃ O ₈ Cl	354.1081	354.1075	1.75	MH-WTP	
204	C ₁₂ H ₁₄ O ₈ Cl ₂	356.0066	356.0059	1.81	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)
205	C ₁₆ H ₁₉ O ₇ Cl	358.0819	358.0811	2.44	MH-WTP	Lavonen et al. (2013)
206	C ₁₇ H ₂₃ O ₆ Cl	358.1183	358.1171	3.48	MH-WTP	Lavonen et al. (2013)
207	C ₁₆ H ₂₁ O ₇ Cl	360.0976	360.0968	2.26	MH-WTP	Lavonen et al. (2013)
208	C ₁₉ H ₃₀ O ₂ Cl ₂	360.1623	360.1624	0.34	MH-WTP	
209	C ₁₅ H ₁₉ O ₈ Cl	362.0768	362.0760	2.26	MH-WTP	Lavonen et al. (2013)
210	C ₁₈ H ₃₁ O ₅ Cl	362.1860	362.1852	2.13	MH-WTP	
211	C ₁₄ H ₁₄ O ₇ Cl ₂	364.0117	364.0112	1.38	MH-WTP	Lavonen et al. (2013), Zhang et al. (2014)
212	C ₁₈ H ₁₇ O ₆ Cl	364.0714	364.0723	2.56	MH-WTP	Lavonen et al. (2013)
213	C ₁₃ H ₂₁ O ₈ Cl	364.0925	364.0912	3.46	MH-WTP	Lavonen et al. (2013)
214	C ₁₆ H ₂₁ O ₃ Cl ₃	366.0556	366.0551	1.53	MH-WTP	
215	C ₁₄ H ₁₉ O ₉ Cl	366.0718	366.0705	3.50	MH-WTP	Lavonen et al. (2013)
216	C ₁₇ H ₁₇ O ₇ Cl	368.0663	368.0653	2.75	MH-WTP	Lavonen et al. (2013)
217	C ₁₃ H ₂₅ O ₈ Cl	368.1238	368.1226	3.25	MH-WTP	
218	C ₁₆ H ₂₉ O ₇ Cl	368.1602	368.1596	1.53	MH-WTP	
219	C ₂₀ H ₂₉ O ₄ Cl	368.1754	368.1760	1.42	BK-WTP	Lavonen et al. (2013)
220	C ₁₄ H ₁₇ O ₅ Cl ₃	370.0142	370.0136	1.65	BK-WTP	
221	C ₁₆ H ₂₅ O ₃ Cl ₃	370.0869	370.0870	0.08	MH-WTP	
222	C ₁₇ H ₃₃ O ₂ Cl ₃	374.1546	374.1549	0.79	MH-WTP	
223	C ₁₅ H ₂₇ O ₄ Cl ₃	376.0975	376.0971	0.97	BK-WTP	
224	C ₁₇ H ₂₅ O ₇ Cl	376.1289	376.1275	3.81	MH-WTP	Lavonen et al. (2013)
225	C ₁₆ H ₃₁ O ₃ Cl ₃	376.1339	376.1332	1.78	BK-WTP	
226	C ₁₆ H ₂₃ O ₈ Cl	378.1081	378.1070	3.06	MH-WTP	Lavonen et al. (2013)
227	C ₁₆ H ₂₇ O ₄ Cl ₃	388.0975	388.0976	0.20	MH-WTP	
228	C ₁₁ H ₁₅ O ₁₃ Cl	390.0201	390.0205	1.02	MH-WTP	
229	C ₁₇ H ₃₃ O ₃ Cl ₃	390.1495	390.1495	0.07	BK-WTP	
230	C ₁₅ H ₃₁ O ₉ Cl	390.1657	390.1670	3.43	MH-WTP	
231	C ₁₄ H ₂₉ O ₁₀ Cl	392.1449	392.1458	2.20	Both WTPs	
232	C ₁₇ H ₂₇ O ₈ Cl	394.1394	394.1387	1.92	MH-WTP	Lavonen et al. (2013)
233	C ₂₁ H ₄₀ O ₂ Cl ₂	394.2405	394.2406	0.26	BK-WTP	
234	C ₁₂ H ₅ O ₉ Cl ₃	397.8999	397.8986	3.39	MH-WTP	
235	C ₁₈ H ₂₉ O ₃ Cl ₃	398.1182	398.1176	1.53	MH-WTP	
236	C ₂₂ H ₂₁ OCl ₃	406.0658	406.0651	1.65	MH-WTP	
237	C ₁₄ H ₂₇ O ₁₁ Cl	406.1242	406.1254	3.05	Both WTPs	
238	C ₁₇ H ₃₃ O ₄ Cl ₃	406.1444	406.1442	0.70	BK-WTP	

No.	DBP formula	Theoretical molecular weight (Da)	Experimental molecular weight (Da)	Mass error (ppm)	Detected in WTP	Also reported in references
239	C ₁₂ H ₂₀ O ₁₁ Cl ₂	410.0383	410.0394	2.75	BK-WTP	
240	C ₁₇ H ₂₅ O ₅ Cl ₃	414.0768	414.0756	2.70	Both WTPs	
241	C ₂₄ H ₂₄ O ₂ Cl ₂	414.1153	414.1135	4.34	MH-WTP	
242	C ₁₈ H ₃₅ O ₄ Cl ₃	418.1444	418.1452	1.69	BK-WTP	
243	C ₁₈ H ₃₅ O ₄ Cl ₃	420.1601	420.1603	0.59	BK-WTP	
244	C ₁₃ H ₁₉ O ₁₄ Cl	434.0463	434.0470	1.55	BK-WTP	
245	C ₂₆ H ₂₆ O ₃ Cl ₂	456.1259	456.1252	1.47	MH-WTP	
246	C ₁₉ H ₂₉ O ₆ Cl ₃	458.1030	458.1043	2.92	Both WTPs	
247	C ₂₄ H ₂₃ O ₇ Cl	458.1132	458.1116	3.48	BK-WTP	
248	C ₂₄ H ₂₄ O ₅ Cl ₂	462.1001	462.0985	3.33	BK-WTP	
249	C ₂₁ H ₃₅ O ₅ Cl ₃	472.1550	472.1563	2.67	MH-WTP	
250	C ₁₅ H ₂₁ O ₁₅ Cl	476.0569	476.0579	2.05	MH-WTP	
251	C ₂₁ H ₃₃ O ₆ Cl ₃	486.1343	486.1356	2.73	MH-WTP	
252	C ₂₁ H ₂₉ O ₇ Cl ₃	498.0979	498.0997	3.64	BK-WTP	

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