

SUPPORTING INFORMATION

for

Study on Transformation of Natural Organic Matter in Source Water during Chlorination and Its Chlorinated Products using Ultrahigh Resolution Mass Spectrometry

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Figures: 14

Tables: 3

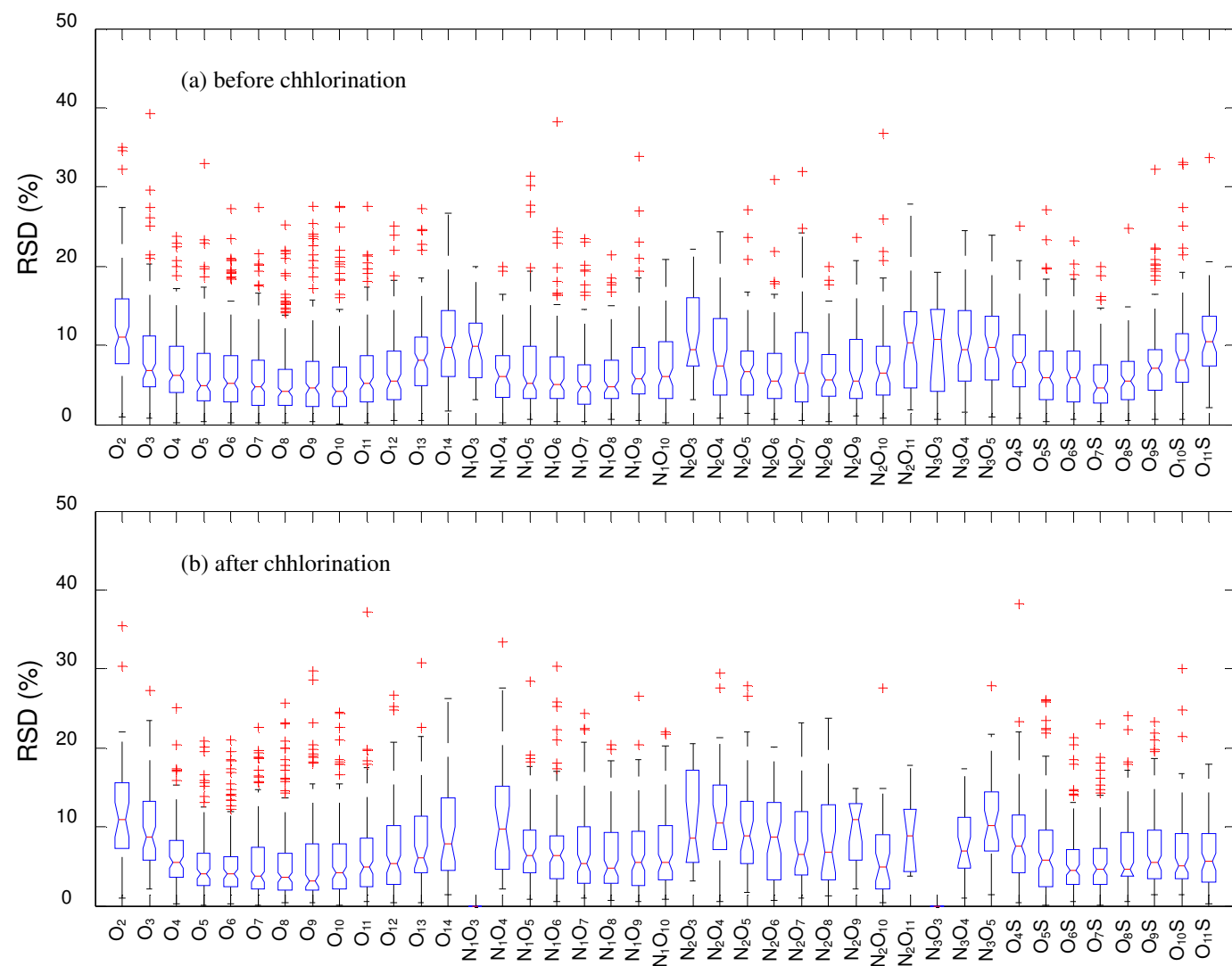


FIGURE S1. Boxplots of RSDs for peak intensities of each molecular class from triplicate measurement of Taihe samples (a) before chlorination and (b) after chlorination. The lower and upper edges of the box represent the 25th and 75th percentile values, respectively. The middle red line represents the median value. The whiskers display the range of data and the red plus symbol represents the outliers.

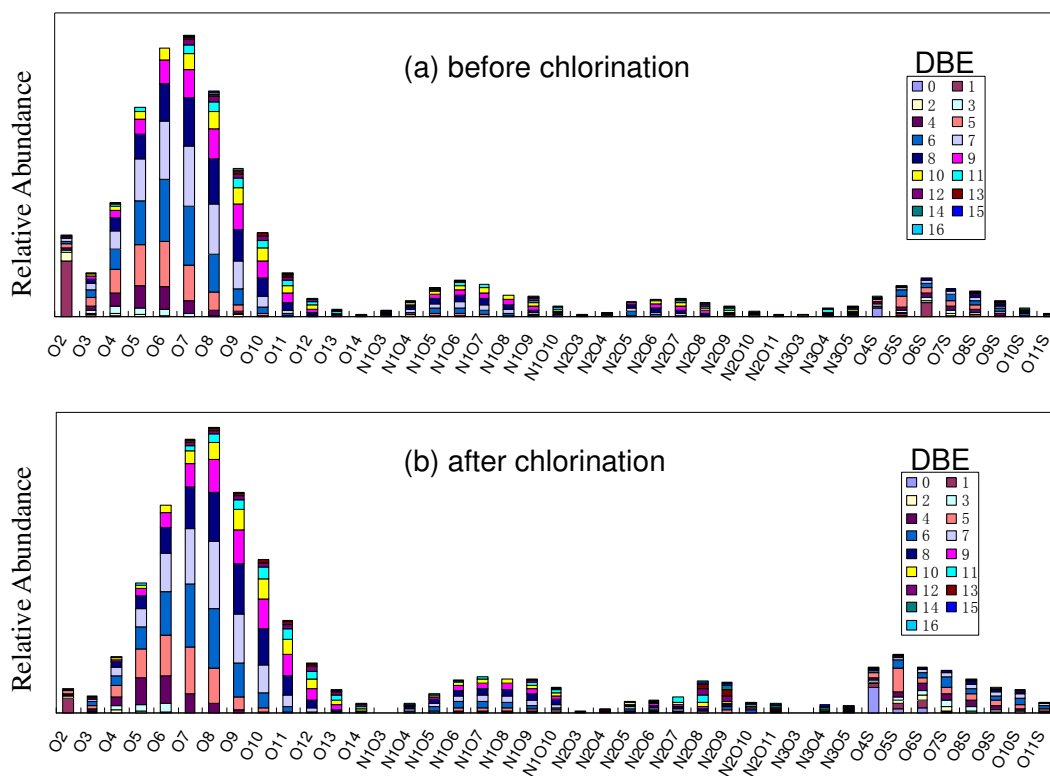


FIGURE S2. Classes analysis for Taihe NOM before and after chlorination.

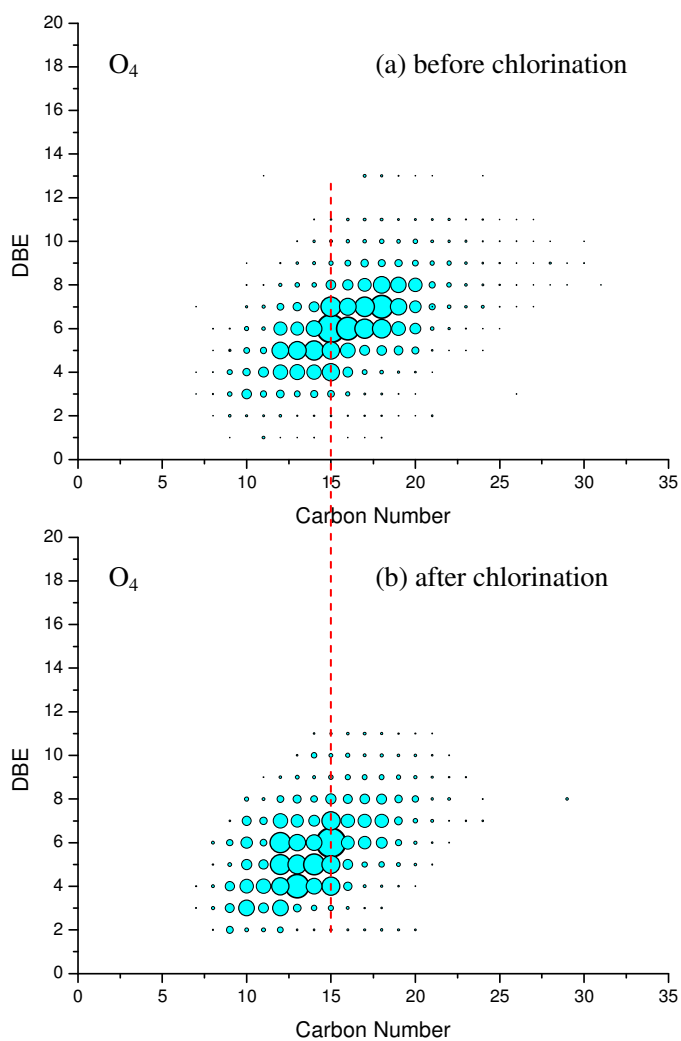


FIGURE S3. Plots of DBE versus the carbon number for the O₄ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

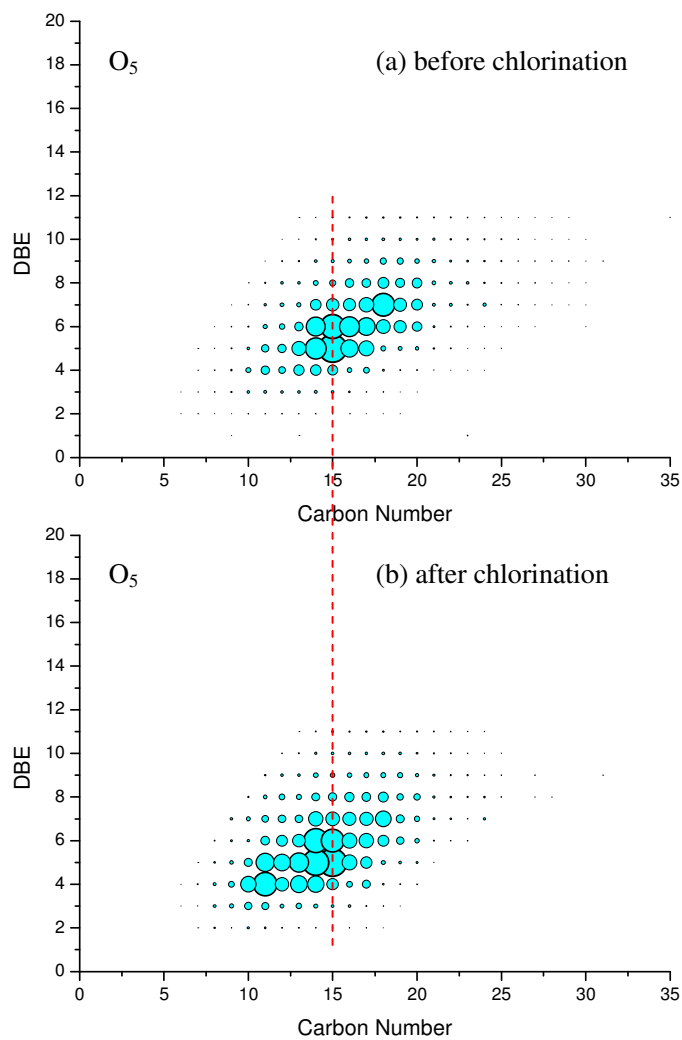


FIGURE S4. Plots of DBE versus the carbon number for the O₅ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

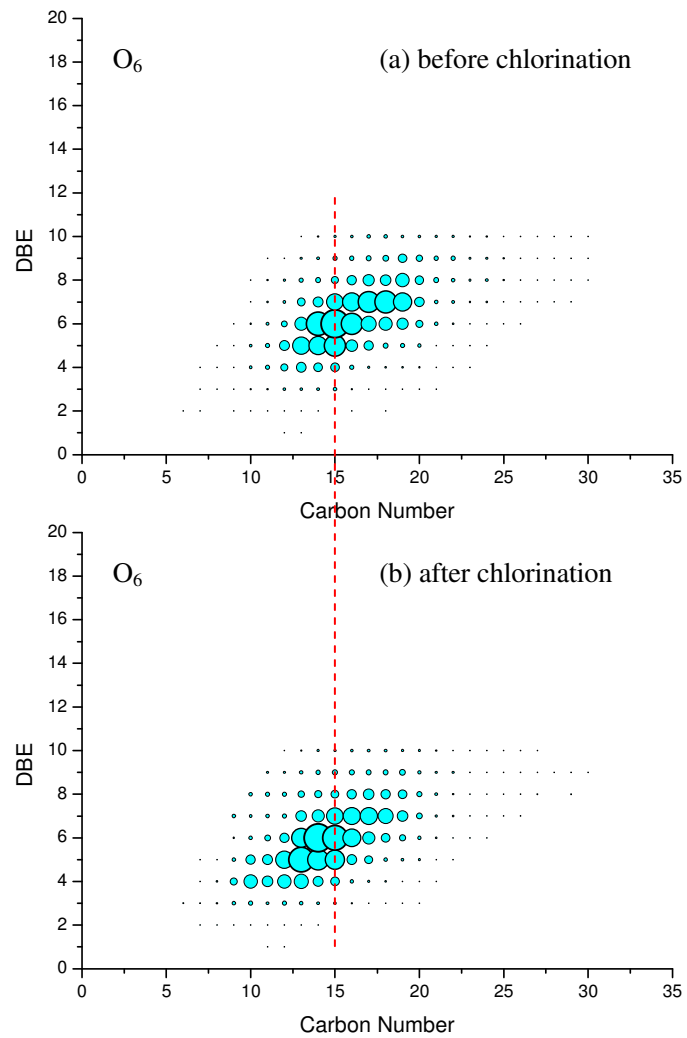


FIGURE S5. Plots of DBE versus the carbon number for the O₆ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

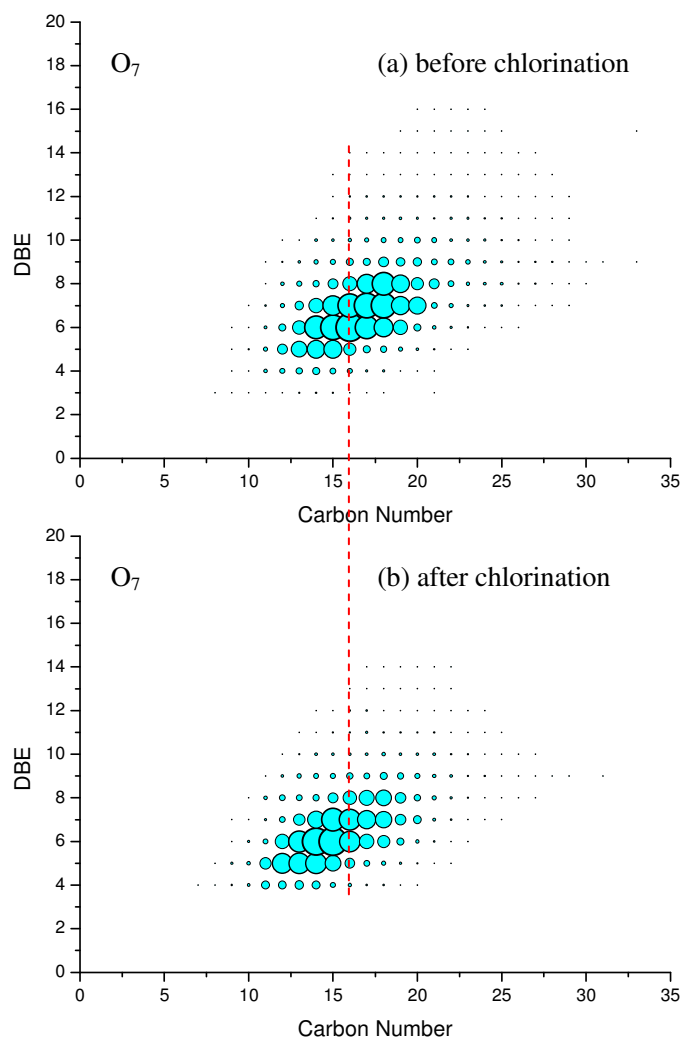


FIGURE S6. Plots of DBE versus the carbon number for the O₇ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

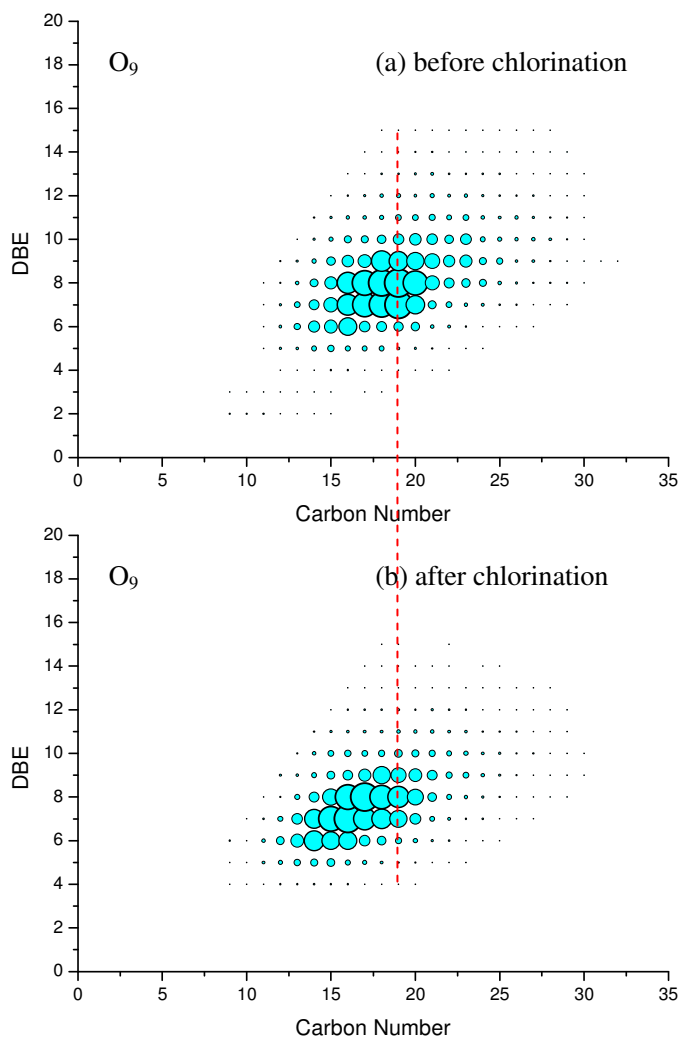


FIGURE S7. Plots of DBE versus the carbon number for the O₉ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

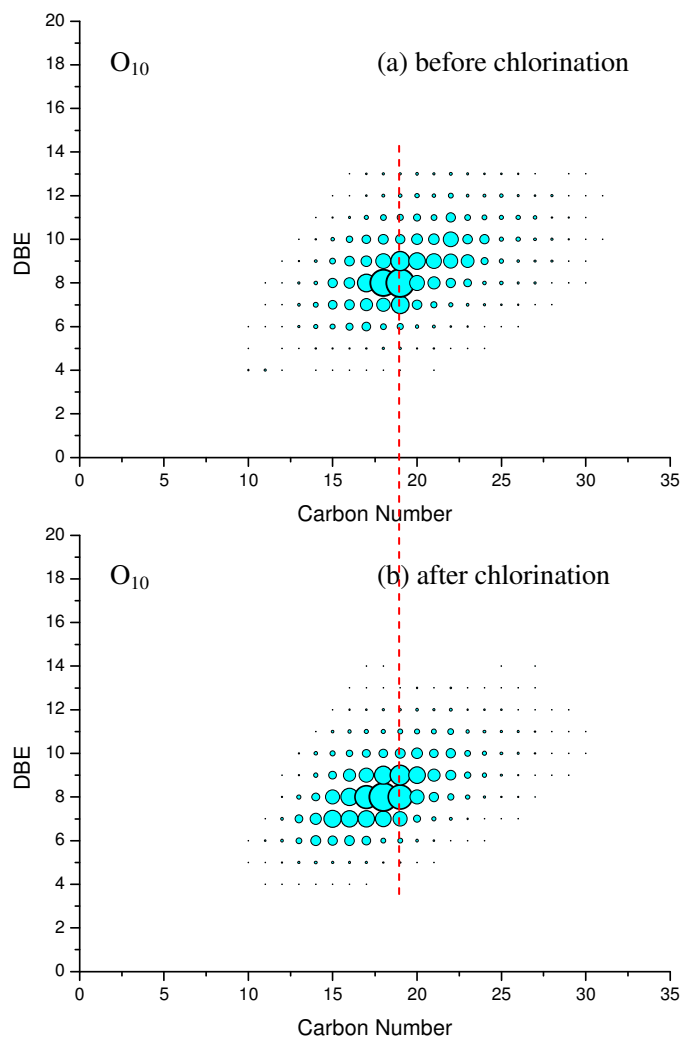


FIGURE S8. Plots of DBE versus the carbon number for the O₁₀ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

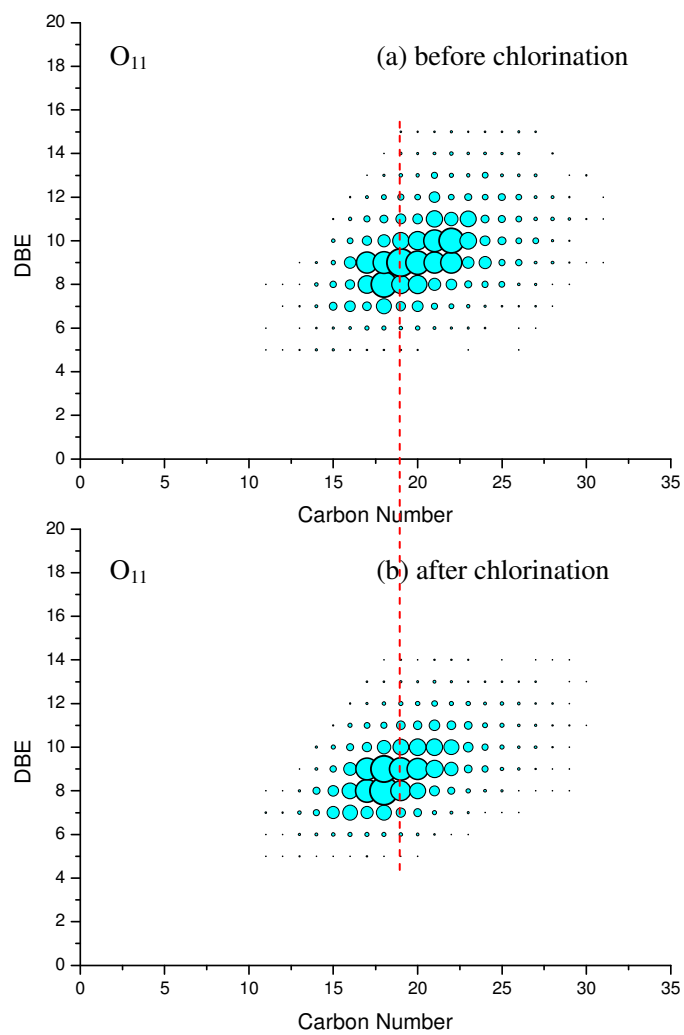


FIGURE S9. Plots of DBE versus the carbon number for the O₁₁ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

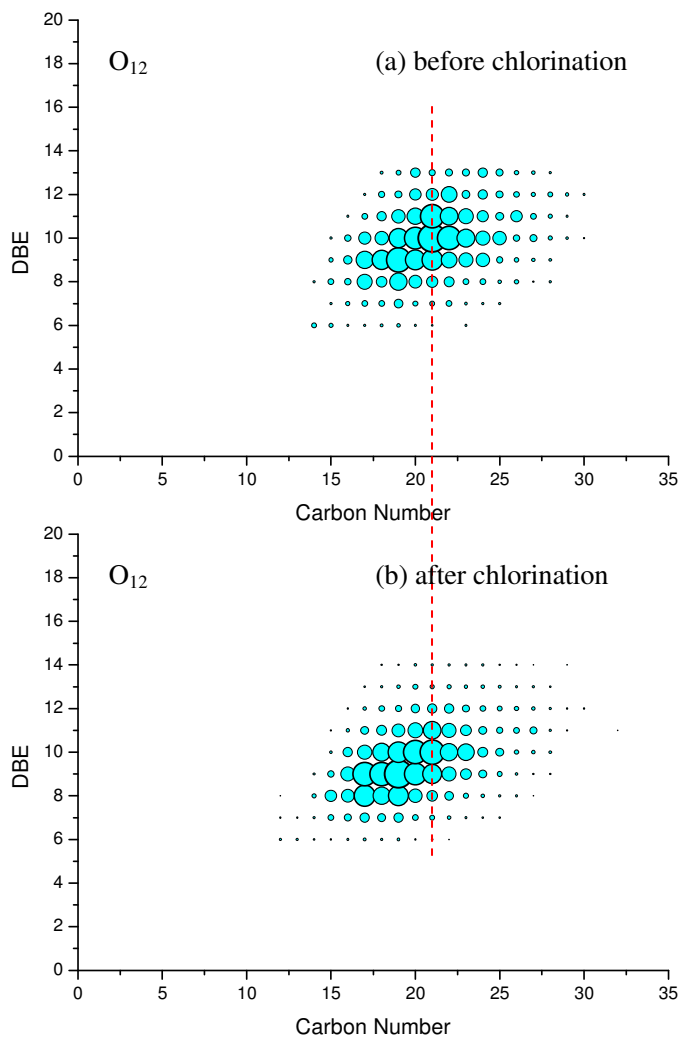


FIGURE S10. Plots of DBE versus the carbon number for the O_{12} C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

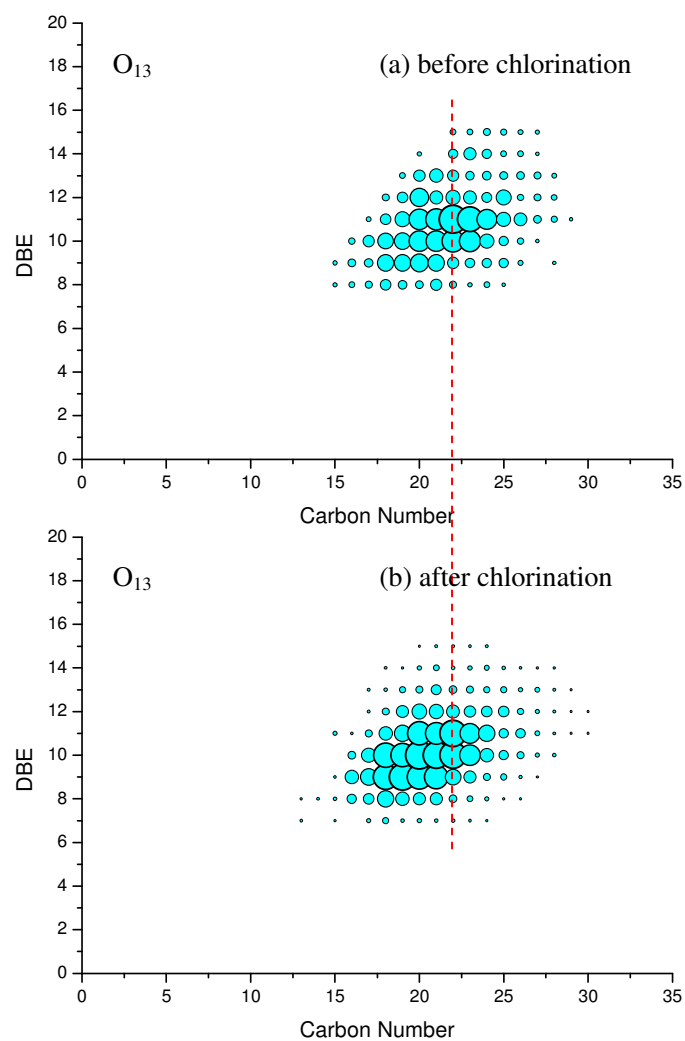


FIGURE S11. Plots of DBE versus the carbon number for the O₁₃ C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

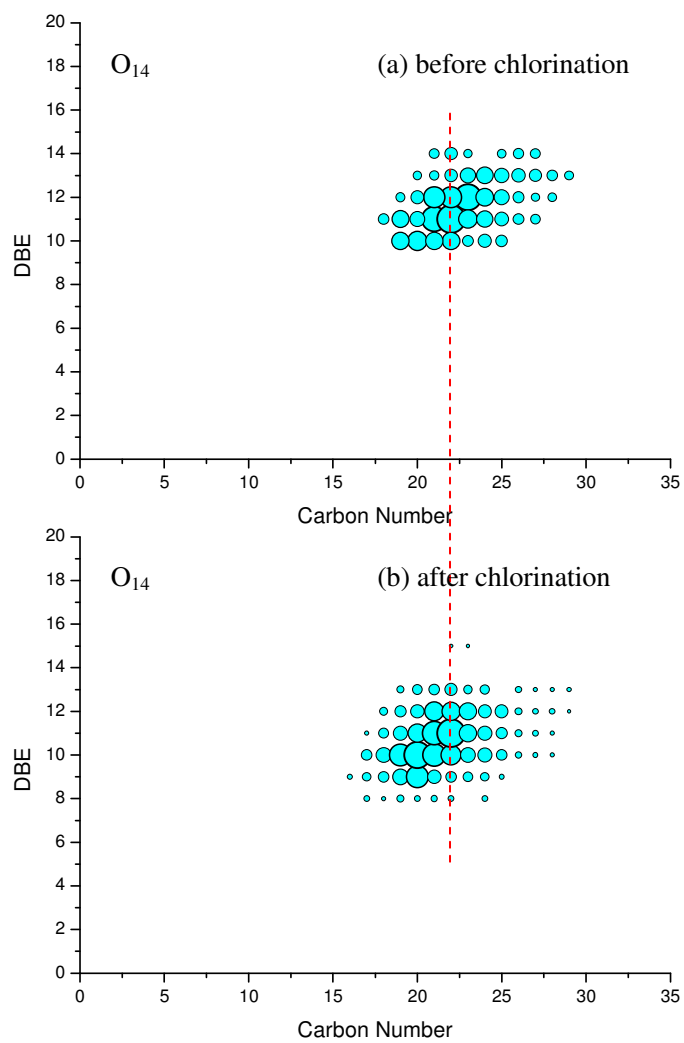


FIGURE S12. Plots of DBE versus the carbon number for the O_{14} C, H, O-only class species in Taihe NOM (a) before chlorination and (b) after chlorination

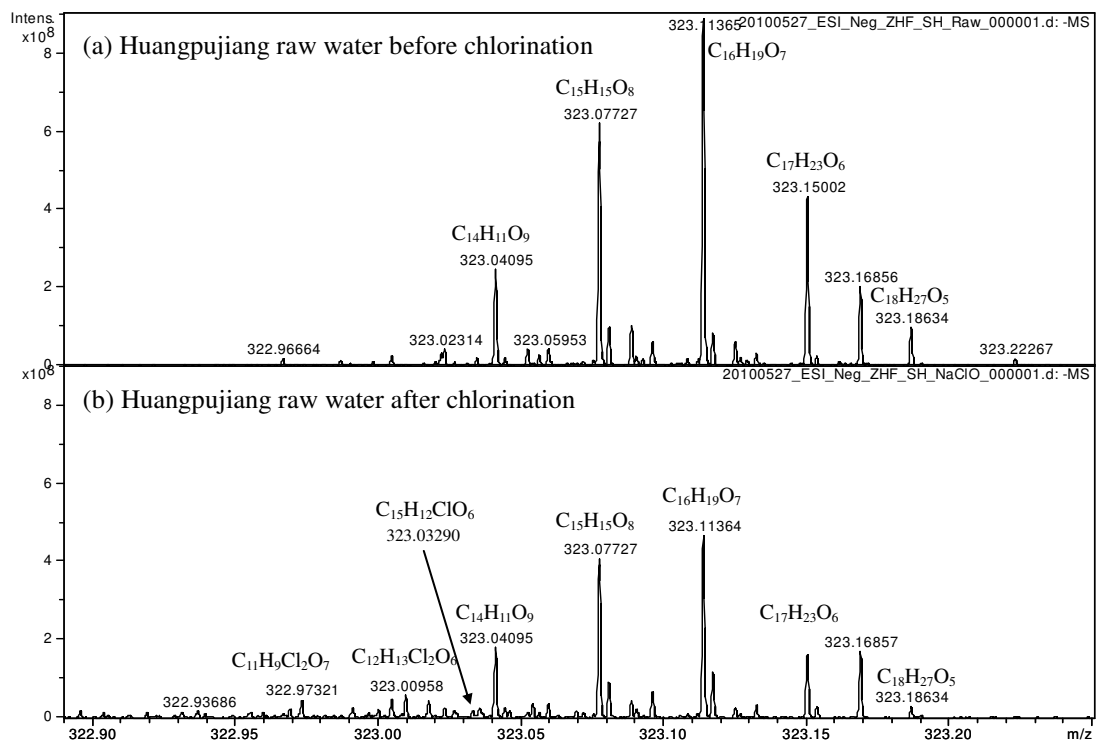


FIGURE S13. Exemplary negative-ion ESI FT-ICR mass spectra for Huangpujiang sample at nominal mass 323 (a) before chlorination (b) after chlorination

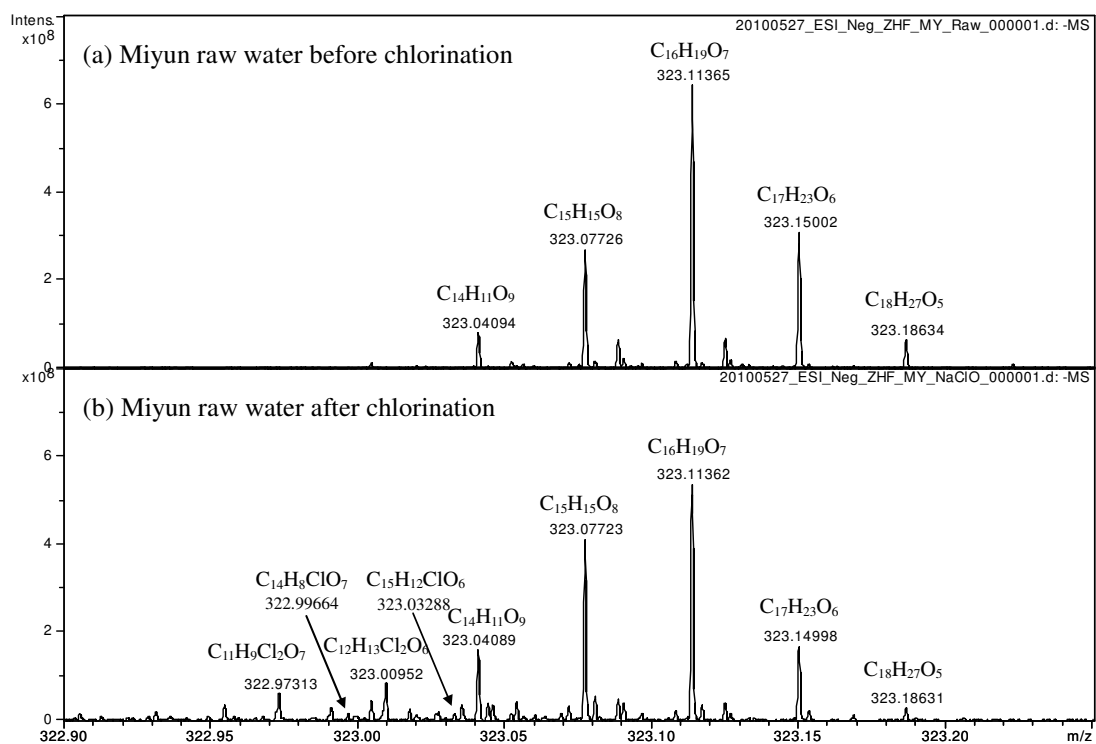


FIGURE S14. Exemplary negative-ion ESI FT-ICR mass spectra for Miyun sample at nominal mass 323 (a) before chlorination (b) after chlorination

Table S1 Carbon number range and DBE range for CHO, CHON and CHOS classes for Taihe samples before and after chlorination.

before chlorination			after chlorination		
class	carbon number range	DBE range	class	carbon number range	DBE range
CHO compounds			CHO compounds		
O ₇	8-33	3-16	O ₈	9-28	4-14
O ₆	6-30	1-10	O ₇	7-31	4-14
O ₈	10-30	3-15	O ₉	9-30	4-15
O ₅	6-30	1-11	O ₆	6-30	1-10
O ₉	9-32	2-15	O ₁₀	10-30	4-14
O ₄	7-31	1-13	O ₅	6-28	2-11
O ₁₀	10-31	4-13	O ₁₁	11-30	5-14
O ₂	9-30	1-10	O ₄	7-29	2-11
O ₃	8-28	1-11	O ₁₂	12-30	6-14
O ₁₁	11-31	5-15	O ₂	9-27	1-8
O ₁₂	14-30	6-13	O ₁₃	13-30	7-15
O ₁₃	15-29	8-15	O ₃	8-22	2-11
O ₁₄	18-29	10-14	O ₁₄	16-29	8-15
CHON compounds			CHON compounds		
N ₁ O ₆	7-26	4-13	N ₁ O ₇	7-25	3-11
N ₁ O ₇	8-28	4-11	N ₁ O ₈	9-24	3-10
N ₁ O ₅	6-25	3-13	N ₁ O ₉	10-26	4-14
N ₁ O ₈	9-26	4-10	N ₁ O ₆	8-24	4-13
N ₁ O ₉	10-29	5-14	N ₂ O ₈	10-28	7-17
N ₂ O ₇	9-25	5-13	N ₂ O ₉	11-28	5-16
N ₂ O ₆	8-27	5-12	N ₁ O ₁₀	11-26	4-13
N ₁ O ₄	7-26	5-13	N ₁ O ₅	7-22	5-13
N ₂ O ₅	7-22	4-12	N ₂ O ₇	9-30	5-12
N ₂ O ₈	11-25	7-14	N ₂ O ₆	8-24	4-12
N ₂ O ₉	11-25	4-14	N ₂ O ₅	7-22	4-15
N ₁ O ₁₀	11-27	4-12	N ₂ O ₁₀	12-28	6-17
N ₃ O ₅	8-26	5-13	N ₂ O ₁₁	13-26	9-16
N ₃ O ₄	7-33	5-14	N ₁ O ₄	7-24	6-16
N ₁ O ₃	8-21	5-11	N ₃ O ₄	7-33	5-15
N ₂ O ₁₀	13-26	6-14	N ₃ O ₅	8-24	5-15
N ₂ O ₄	7-18	4-13	N ₂ O ₄	8-21	7-15
N ₃ O ₃	7-29	9-14	N ₂ O ₃	9-30	8-16
N ₂ O ₃	7-25	6-13			
N ₂ O ₁₁	13-24	4-12			
CHOS compounds			CHOS compounds		
O ₆ S	7-27	1-8	O ₅ S	6-32	0-11
O ₅ S	6-24	0-11	O ₄ S	6-28	0-10
O ₇ S	7-28	1-8	O ₆ S	7-26	0-9
O ₈ S	8-29	1-13	O ₇ S	7-24	0-8
O ₄ S	7-28	0-11	O ₈ S	8-24	2-13
O ₉ S	9-29	1-11	O ₉ S	9-25	2-10
O ₁₀ S	12-29	5-10	O ₁₀ S	10-24	3-11
O ₁₁ S	11-27	4-9	O ₁₁ S	11-23	4-10

* Classes in each elemental group (CHO, CHON and CHOS) were listed in order of decreasing abundance

Table S2 Molecular formulas for newly formed chlorine-containing products detected in chlorinated Taihe sample

one chlorine-containing products			
formula (M-H) ⁻	measured mass	theoretical mass	error (ppm)
C ₈ H ₆ ClO ₃	185.00110	185.00110	0
C ₈ H ₈ ClO ₃	187.01682	187.01675	0.39
C ₈ H ₁₀ ClO ₃	189.03241	189.03240	0.07
C ₉ H ₈ ClO ₃	199.01679	199.01675	0.22
C ₉ H ₁₂ ClO ₃	203.04811	203.04805	0.31
C ₉ H ₁₄ ClO ₃	205.06361	205.06370	-0.42
C ₁₀ H ₆ ClO ₃	209.00113	209.00110	0.16
C ₁₀ H ₈ ClO ₃	211.01671	211.01675	-0.18
C ₁₀ H ₁₀ ClO ₃	213.03239	213.03240	-0.03
C ₁₀ H ₁₂ ClO ₃	215.04802	215.04805	-0.13
C ₁₀ H ₁₄ ClO ₃	217.06367	217.06370	-0.12
C ₁₀ H ₁₆ ClO ₃	219.07934	219.07935	-0.03
C ₁₀ H ₁₈ ClO ₃	221.09501	221.09500	0.06
C ₁₁ H ₈ ClO ₃	223.01676	223.01675	0.06
C ₁₁ H ₁₀ ClO ₃	225.03233	225.03240	-0.30
C ₁₁ H ₁₂ ClO ₃	227.04807	227.04805	0.10
C ₁₁ H ₁₄ ClO ₃	229.06373	229.06370	0.14
C ₁₁ H ₁₆ ClO ₃	231.07938	231.07935	0.14
C ₁₂ H ₁₀ ClO ₃	237.03232	237.03240	-0.32
C ₁₂ H ₁₂ ClO ₃	239.04795	239.04805	-0.41
C ₁₂ H ₁₄ ClO ₃	241.06376	241.06370	0.26
C ₁₂ H ₁₈ ClO ₃	245.09494	245.09500	-0.23
C ₁₂ H ₂₀ ClO ₃	247.11059	247.11065	-0.23
C ₁₃ H ₁₄ ClO ₃	253.06381	253.06370	0.45
C ₁₃ H ₁₆ ClO ₃	255.07944	255.07935	0.36
C ₁₃ H ₁₈ ClO ₃	257.09500	257.09500	0
C ₁₃ H ₂₀ ClO ₃	259.11055	259.11065	-0.37
C ₁₃ H ₂₂ ClO ₃	261.12623	261.12630	-0.26
C ₁₄ H ₁₄ ClO ₃	265.06359	265.06370	-0.40
C ₁₄ H ₁₆ ClO ₃	267.07939	267.07935	0.16
C ₁₄ H ₁₈ ClO ₃	269.09501	269.09500	0.05
C ₁₄ H ₂₀ ClO ₃	271.11057	271.11065	-0.28
C ₁₄ H ₂₂ ClO ₃	273.12639	273.12630	0.34
C ₁₄ H ₂₄ ClO ₃	275.14198	275.14195	0.12
C ₁₄ H ₂₆ ClO ₃	277.15766	277.15760	0.23
C ₁₅ H ₁₈ ClO ₃	281.09493	281.09500	-0.24
C ₁₅ H ₂₀ ClO ₃	283.11057	283.11065	-0.27
C ₁₅ H ₂₂ ClO ₃	285.12639	285.12630	0.33
C ₁₅ H ₂₄ ClO ₃	287.14184	287.14195	-0.37
C ₁₅ H ₂₆ ClO ₃	289.15750	289.15760	-0.34
C ₁₆ H ₂₀ ClO ₃	295.11075	295.11065	0.35
C ₁₆ H ₂₄ ClO ₃	299.14181	299.14195	-0.46
C ₇ H ₄ ClO ₄	186.98043	186.98036	0.36
C ₇ H ₆ ClO ₄	188.99604	188.99601	0.15

C ₇ H ₈ ClO ₄	191.01166	191.01166	0
C ₈ H ₄ ClO ₄	198.98036	198.98036	0
C ₈ H ₈ ClO ₄	203.01176	203.01166	0.48
C ₈ H ₁₀ ClO ₄	205.02730	205.02731	-0.06
C ₉ H ₄ ClO ₄	210.98039	210.98036	0.13
C ₉ H ₆ ClO ₄	212.99599	212.99601	-0.10
C ₉ H ₈ ClO ₄	215.01164	215.01166	-0.10
C ₉ H ₁₀ ClO ₄	217.02728	217.02731	-0.15
C ₉ H ₁₂ ClO ₄	219.04294	219.04296	-0.10
C ₉ H ₁₄ ClO ₄	221.05867	221.05861	0.26
C ₁₀ H ₄ ClO ₄	222.98037	222.98036	0.04
C ₁₀ H ₆ ClO ₄	224.99597	224.99601	-0.19
C ₁₀ H ₈ ClO ₄	227.01174	227.01166	0.34
C ₁₀ H ₁₀ ClO ₄	229.02729	229.02731	-0.10
C ₁₀ H ₁₂ ClO ₄	231.04303	231.04296	0.29
C ₁₀ H ₁₄ ClO ₄	233.05858	233.05861	-0.14
C ₁₁ H ₆ ClO ₄	236.99600	236.99601	-0.05
C ₁₁ H ₈ ClO ₄	239.01163	239.01166	-0.13
C ₁₁ H ₁₀ ClO ₄	241.02731	241.02731	0
C ₁₁ H ₁₂ ClO ₄	243.04309	243.04296	0.53
C ₁₁ H ₁₄ ClO ₄	245.05871	245.05861	0.40
C ₁₁ H ₁₆ ClO ₄	247.07430	247.07426	0.15
C ₁₁ H ₁₈ ClO ₄	249.08993	249.08991	0.07
C ₁₁ H ₂₀ ClO ₄	251.10569	251.10556	0.51
C ₁₂ H ₁₀ ClO ₄	253.02743	253.02731	0.47
C ₁₂ H ₁₂ ClO ₄	255.04307	255.04296	0.42
C ₁₂ H ₁₄ ClO ₄	257.05860	257.05861	-0.05
C ₁₂ H ₁₆ ClO ₄	259.07419	259.07426	-0.28
C ₁₂ H ₁₈ ClO ₄	261.08990	261.08991	-0.05
C ₁₂ H ₂₀ ClO ₄	263.10569	263.10556	0.49
C ₁₃ H ₁₀ ClO ₄	265.02724	265.02731	-0.27
C ₁₃ H ₁₂ ClO ₄	267.04302	267.04296	0.22
C ₁₃ H ₁₄ ClO ₄	269.05858	269.05861	-0.12
C ₁₃ H ₁₆ ClO ₄	271.07422	271.07426	-0.15
C ₁₃ H ₁₈ ClO ₄	273.08993	273.08991	0.07
C ₁₃ H ₂₀ ClO ₄	275.10549	275.10556	-0.26
C ₁₃ H ₂₂ ClO ₄	277.12116	277.12121	-0.19
C ₁₄ H ₁₄ ClO ₄	281.05851	281.05861	-0.36
C ₁₄ H ₁₆ ClO ₄	283.07425	283.07426	-0.04
C ₁₄ H ₁₈ ClO ₄	285.09003	285.08991	0.41
C ₁₄ H ₂₀ ClO ₄	287.10548	287.10556	-0.29
C ₁₄ H ₂₂ ClO ₄	289.12108	289.12121	-0.46
C ₁₄ H ₂₄ ClO ₄	291.13685	291.13686	-0.04
C ₁₅ H ₁₆ ClO ₄	295.07437	295.07426	0.37
C ₁₅ H ₁₈ ClO ₄	297.08995	297.08991	0.13
C ₁₅ H ₂₀ ClO ₄	299.10551	299.10556	-0.17
C ₁₅ H ₂₂ ClO ₄	301.12110	301.12121	-0.37
C ₁₅ H ₂₄ ClO ₄	303.13674	303.13686	-0.40

C ₁₆ H ₁₈ ClO ₄	309.08987	309.08991	-0.14
C ₁₆ H ₂₀ ClO ₄	311.10561	311.10556	0.15
C ₁₆ H ₂₂ ClO ₄	313.12134	313.12121	0.41
C ₁₆ H ₂₆ ClO ₄	317.15247	317.15251	-0.13
C ₁₆ H ₂₈ ClO ₄	319.16803	319.16816	-0.41
C ₁₇ H ₂₀ ClO ₄	323.10564	323.10556	0.24
C ₁₇ H ₂₂ ClO ₄	325.12137	325.12121	0.49
C ₁₇ H ₂₄ ClO ₄	327.13672	327.13686	-0.43
C ₁₇ H ₂₆ ClO ₄	329.15230	329.15251	-0.64
C ₁₇ H ₂₈ ClO ₄	331.16819	331.16816	0.08
C ₁₈ H ₂₄ ClO ₄	339.13678	339.13686	-0.24
C ₁₈ H ₂₆ ClO ₄	341.15237	341.15251	-0.42
C ₁₈ H ₂₈ ClO ₄	343.16831	343.16816	0.43
C ₁₈ H ₃₀ ClO ₄	345.18363	345.18381	-0.53
C ₁₉ H ₂₆ ClO ₄	353.15231	353.15251	-0.57
C ₁₉ H ₂₈ ClO ₄	355.16839	355.16816	0.64
C ₁₉ H ₃₀ ClO ₄	357.18355	357.18381	-0.73
C ₂₀ H ₂₈ ClO ₄	367.16801	367.16816	-0.41
C ₂₀ H ₃₀ ClO ₄	369.18408	369.18381	0.73
C ₆ H ₄ ClO ₅	190.97530	190.97528	0.12
C ₇ H ₄ ClO ₅	202.97539	202.97528	0.56
C ₇ H ₆ ClO ₅	204.99092	204.99093	-0.03
C ₈ H ₄ ClO ₅	214.97526	214.97528	-0.08
C ₈ H ₆ ClO ₅	216.99090	216.99093	-0.12
C ₈ H ₈ ClO ₅	219.00659	219.00658	0.06
C ₈ H ₁₀ ClO ₅	221.02229	221.02223	0.29
C ₉ H ₄ ClO ₅	226.97536	226.97528	0.37
C ₉ H ₆ ClO ₅	228.99090	228.99093	-0.12
C ₉ H ₈ ClO ₅	231.00666	231.00658	0.36
C ₉ H ₁₀ ClO ₅	233.02219	233.02223	-0.16
C ₁₀ H ₄ ClO ₅	238.97524	238.97528	-0.15
C ₁₀ H ₆ ClO ₅	240.99093	240.99093	0
C ₁₀ H ₈ ClO ₅	243.00669	243.00658	0.47
C ₁₀ H ₁₀ ClO ₅	245.02234	245.02223	0.46
C ₁₀ H ₁₂ ClO ₅	247.03795	247.03788	0.30
C ₁₀ H ₁₄ ClO ₅	249.05362	249.05353	0.37
C ₁₀ H ₁₆ ClO ₅	251.06926	251.06918	0.33
C ₁₁ H ₆ ClO ₅	252.99101	252.99093	0.33
C ₁₁ H ₈ ClO ₅	255.00661	255.00658	0.13
C ₁₁ H ₁₀ ClO ₅	257.02218	257.02223	-0.18
C ₁₁ H ₁₂ ClO ₅	259.03780	259.03788	-0.30
C ₁₁ H ₁₄ ClO ₅	261.05357	261.05353	0.16
C ₁₁ H ₁₆ ClO ₅	263.06931	263.06918	0.51
C ₁₂ H ₆ ClO ₅	264.99086	264.99093	-0.25
C ₁₂ H ₈ ClO ₅	267.00668	267.00658	0.39
C ₁₂ H ₁₀ ClO ₅	269.02218	269.02223	-0.17
C ₁₂ H ₁₂ ClO ₅	271.03787	271.03788	-0.03
C ₁₂ H ₁₄ ClO ₅	273.05350	273.05353	-0.10

C ₁₂ H ₁₆ ClO ₅	275.06918	275.06918	0
C ₁₂ H ₁₈ ClO ₅	277.08476	277.08483	-0.24
C ₁₂ H ₂₀ ClO ₅	279.10060	279.10048	0.44
C ₁₃ H ₁₀ ClO ₅	281.02219	281.02223	-0.13
C ₁₃ H ₁₂ ClO ₅	283.03782	283.03788	-0.20
C ₁₃ H ₁₄ ClO ₅	285.05366	285.05353	0.47
C ₁₃ H ₁₆ ClO ₅	287.06913	287.06918	-0.16
C ₁₃ H ₁₈ ClO ₅	289.08468	289.08483	-0.51
C ₁₃ H ₂₀ ClO ₅	291.10041	291.10048	-0.23
C ₁₃ H ₂₂ ClO ₅	293.11626	293.11613	0.45
C ₁₄ H ₁₂ ClO ₅	295.03804	295.03788	0.55
C ₁₄ H ₁₄ ClO ₅	297.05362	297.05353	0.31
C ₁₄ H ₁₆ ClO ₅	299.06914	299.06918	-0.12
C ₁₄ H ₁₈ ClO ₅	301.08473	301.08483	-0.32
C ₁₄ H ₂₀ ClO ₅	303.10038	303.10048	-0.32
C ₁₄ H ₂₂ ClO ₅	305.11603	305.11613	-0.32
C ₁₄ H ₂₄ ClO ₅	307.13170	307.13178	-0.25
C ₁₅ H ₁₄ ClO ₅	309.05352	309.05353	-0.02
C ₁₅ H ₁₆ ClO ₅	311.06925	311.06918	0.23
C ₁₅ H ₁₈ ClO ₅	313.08498	313.08483	0.49
C ₁₅ H ₂₂ ClO ₅	317.11609	317.11613	-0.12
C ₁₅ H ₂₄ ClO ₅	319.13162	319.13178	-0.49
C ₁₅ H ₂₆ ClO ₅	321.14722	321.14743	-0.64
C ₁₆ H ₁₆ ClO ₅	323.06926	323.06918	0.26
C ₁₆ H ₁₈ ClO ₅	325.08497	325.08483	0.44
C ₁₆ H ₂₀ ClO ₅	327.10032	327.10048	-0.48
C ₁₆ H ₂₂ ClO ₅	329.11591	329.11613	-0.66
C ₁₆ H ₂₄ ClO ₅	331.13185	331.13178	0.22
C ₁₆ H ₂₆ ClO ₅	333.14743	333.14743	0
C ₁₆ H ₂₈ ClO ₅	335.16282	335.16308	-0.77
C ₁₇ H ₂₀ ClO ₅	339.10035	339.10048	-0.37
C ₁₇ H ₂₂ ClO ₅	341.11606	341.11613	-0.20
C ₁₇ H ₂₄ ClO ₅	343.13193	343.13178	0.45
C ₁₇ H ₂₆ ClO ₅	345.14719	345.14743	-0.69
C ₁₇ H ₂₈ ClO ₅	347.16328	347.16308	0.58
C ₁₈ H ₂₂ ClO ₅	353.11591	353.11613	-0.61
C ₁₈ H ₂₄ ClO ₅	355.13202	355.13178	0.68
C ₁₈ H ₂₆ ClO ₅	357.14723	357.14743	-0.55
C ₁₈ H ₂₈ ClO ₅	359.16329	359.16308	0.59
C ₁₉ H ₂₂ ClO ₅	365.11642	365.11613	0.80
C ₁₉ H ₂₄ ClO ₅	367.13159	367.13178	-0.51
C ₁₉ H ₂₆ ClO ₅	369.14762	369.14743	0.52
C ₁₉ H ₂₈ ClO ₅	371.16314	371.16308	0.17
C ₁₉ H ₃₀ ClO ₅	373.17850	373.17873	-0.61
C ₁₉ H ₃₂ ClO ₅	375.19448	375.19438	0.27
C ₂₀ H ₂₆ ClO ₅	381.14755	381.14743	0.32
C ₂₀ H ₂₈ ClO ₅	383.16344	383.16308	0.95
C ₂₀ H ₃₀ ClO ₅	385.17862	385.17873	-0.28

C ₂₀ H ₃₄ ClO ₅	389.20984	389.21003	-0.48
C ₂₁ H ₃₀ ClO ₅	397.17865	397.17873	-0.19
C ₂₁ H ₃₂ ClO ₅	399.19410	399.19438	-0.69
C ₇ H ₄ ClO ₆	218.97024	218.97019	0.22
C ₇ H ₆ ClO ₆	220.98592	220.98584	0.35
C ₈ H ₄ ClO ₆	230.97030	230.97019	0.47
C ₈ H ₆ ClO ₆	232.98580	232.98584	-0.18
C ₉ H ₄ ClO ₆	242.97019	242.97019	0
C ₉ H ₆ ClO ₆	244.98597	244.98584	0.52
C ₉ H ₈ ClO ₆	247.00160	247.00149	0.44
C ₉ H ₁₀ ClO ₆	249.01724	249.01714	0.39
C ₉ H ₁₂ ClO ₆	251.03289	251.03279	0.39
C ₁₀ H ₄ ClO ₆	254.97020	254.97019	0.03
C ₁₀ H ₆ ClO ₆	256.98579	256.98584	-0.20
C ₁₀ H ₈ ClO ₆	259.00141	259.00149	-0.32
C ₁₀ H ₁₀ ClO ₆	261.01722	261.01714	0.30
C ₁₀ H ₁₂ ClO ₆	263.03288	263.03279	0.33
C ₁₁ H ₄ ClO ₆	266.97029	266.97019	0.37
C ₁₁ H ₆ ClO ₆	268.98577	268.98584	-0.27
C ₁₁ H ₈ ClO ₆	271.00154	271.00149	0.18
C ₁₁ H ₁₀ ClO ₆	273.01711	273.01714	-0.12
C ₁₁ H ₁₂ ClO ₆	275.03284	275.03279	0.17
C ₁₁ H ₁₄ ClO ₆	277.04836	277.04844	-0.30
C ₁₁ H ₁₆ ClO ₆	279.06420	279.06409	0.39
C ₁₂ H ₆ ClO ₆	280.98584	280.98584	0
C ₁₂ H ₈ ClO ₆	283.00144	283.00149	-0.18
C ₁₂ H ₁₀ ClO ₆	285.01730	285.01714	0.55
C ₁₂ H ₁₂ ClO ₆	287.03278	287.03279	-0.04
C ₁₂ H ₁₄ ClO ₆	289.04830	289.04844	-0.49
C ₁₂ H ₁₆ ClO ₆	291.06400	291.06409	-0.32
C ₁₂ H ₁₈ ClO ₆	293.07983	293.07974	0.30
C ₁₃ H ₈ ClO ₆	295.00168	295.00149	0.64
C ₁₃ H ₁₀ ClO ₆	297.01727	297.01714	0.43
C ₁₃ H ₁₂ ClO ₆	299.03279	299.03279	-0.01
C ₁₃ H ₁₄ ClO ₆	301.04839	301.04844	-0.17
C ₁₃ H ₁₆ ClO ₆	303.06401	303.06409	-0.27
C ₁₃ H ₁₈ ClO ₆	305.07965	305.07974	-0.30
C ₁₃ H ₂₀ ClO ₆	307.09532	307.09539	-0.23
C ₁₄ H ₁₀ ClO ₆	309.01726	309.01714	0.38
C ₁₄ H ₁₂ ClO ₆	311.03294	311.03279	0.48
C ₁₄ H ₁₄ ClO ₆	313.04859	313.04844	0.47
C ₁₄ H ₁₈ ClO ₆	317.07966	317.07974	-0.26
C ₁₄ H ₂₀ ClO ₆	319.09521	319.09539	-0.57
C ₁₄ H ₂₂ ClO ₆	321.11083	321.11104	-0.66
C ₁₅ H ₁₂ ClO ₆	323.03292	323.03279	0.40
C ₁₅ H ₁₄ ClO ₆	325.04861	325.04844	0.52
C ₁₅ H ₁₆ ClO ₆	327.06392	327.06409	-0.53
C ₁₅ H ₁₈ ClO ₆	329.07954	329.07974	-0.61

$C_{15}H_{20}ClO_6$	331.09552	331.09539	0.39
$C_{15}H_{22}ClO_6$	333.11100	333.11104	-0.13
$C_{15}H_{24}ClO_6$	335.12645	335.12669	-0.72
$C_{15}H_{26}ClO_6$	337.14246	337.14234	0.35
$C_{16}H_{16}ClO_6$	339.06392	339.06409	-0.51
$C_{16}H_{18}ClO_6$	341.07970	341.07974	-0.12
$C_{16}H_{20}ClO_6$	343.09549	343.09539	0.29
$C_{16}H_{22}ClO_6$	345.11083	345.11104	-0.61
$C_{16}H_{24}ClO_6$	347.12687	347.12669	0.51
$C_{16}H_{26}ClO_6$	349.14207	349.14234	-0.78
$C_{16}H_{28}ClO_6$	351.15826	351.15799	0.76
$C_{17}H_{18}ClO_6$	353.07952	353.07974	-0.63
$C_{17}H_{20}ClO_6$	355.09558	355.09539	0.53
$C_{17}H_{22}ClO_6$	357.11082	357.11104	-0.62
$C_{17}H_{24}ClO_6$	359.12683	359.12669	0.38
$C_{17}H_{26}ClO_6$	361.14220	361.14234	-0.39
$C_{17}H_{28}ClO_6$	363.15796	363.15799	-0.09
$C_{18}H_{18}ClO_6$	365.08002	365.07974	0.76
$C_{18}H_{20}ClO_6$	367.09519	367.09539	-0.55
$C_{18}H_{22}ClO_6$	369.11118	369.11104	0.37
$C_{18}H_{24}ClO_6$	371.12685	371.12669	0.43
$C_{18}H_{26}ClO_6$	373.14212	373.14234	-0.59
$C_{18}H_{28}ClO_6$	375.15823	375.15799	0.63
$C_{18}H_{30}ClO_6$	377.17384	377.17364	0.52
$C_{19}H_{22}ClO_6$	381.11095	381.11104	-0.24
$C_{19}H_{24}ClO_6$	383.12699	383.12669	0.78
$C_{19}H_{26}ClO_6$	385.14238	385.14234	0.10
$C_{19}H_{28}ClO_6$	387.15775	387.15799	-0.63
$C_{19}H_{30}ClO_6$	389.17359	389.17364	-0.13
$C_{19}H_{32}ClO_6$	391.18954	391.18929	0.63
$C_{20}H_{24}ClO_6$	395.12661	395.12669	-0.21
$C_{20}H_{26}ClO_6$	397.14214	397.14234	-0.51
$C_{20}H_{28}ClO_6$	399.15783	399.15799	-0.41
$C_{20}H_{30}ClO_6$	401.17370	401.17364	0.14
$C_{20}H_{32}ClO_6$	403.18942	403.18929	0.32
$C_{21}H_{26}ClO_6$	409.14229	409.14234	-0.13
$C_{21}H_{28}ClO_6$	411.15793	411.15799	-0.15
$C_{21}H_{30}ClO_6$	413.17353	413.17364	-0.27
$C_{21}H_{32}ClO_6$	415.18912	415.18929	-0.41
$C_{21}H_{34}ClO_6$	417.20492	417.20494	-0.05
$C_{22}H_{28}ClO_6$	423.15816	423.15799	0.40
$C_{22}H_{30}ClO_6$	425.17400	425.17364	0.84
$C_{22}H_{32}ClO_6$	427.18960	427.18929	0.72
$C_{23}H_{30}ClO_6$	437.17385	437.17364	0.48
$C_{23}H_{32}ClO_6$	439.18962	439.18929	0.75
$C_{24}H_{32}ClO_6$	451.18925	451.18929	-0.09
$C_{24}H_{34}ClO_6$	453.20488	453.20494	-0.14
$C_8H_4ClO_7$	246.96520	246.96511	0.38

C ₈ H ₆ ClO ₇	248.98088	248.98076	0.49
C ₈ H ₈ ClO ₇	250.99653	250.99641	0.49
C ₉ H ₄ ClO ₇	258.96510	258.96511	-0.03
C ₉ H ₆ ClO ₇	260.98087	260.98076	0.43
C ₉ H ₈ ClO ₇	262.99643	262.99641	0.09
C ₁₀ H ₄ ClO ₇	270.96517	270.96511	0.23
C ₁₀ H ₆ ClO ₇	272.98069	272.98076	-0.25
C ₁₀ H ₈ ClO ₇	274.99649	274.99641	0.30
C ₁₀ H ₁₀ ClO ₇	277.01199	277.01206	-0.24
C ₁₀ H ₁₂ ClO ₇	279.02784	279.02771	0.48
C ₁₁ H ₄ ClO ₇	282.96505	282.96511	-0.20
C ₁₁ H ₆ ClO ₇	284.98091	284.98076	0.54
C ₁₁ H ₈ ClO ₇	286.99645	286.99641	0.15
C ₁₁ H ₁₀ ClO ₇	289.01192	289.01206	-0.47
C ₁₁ H ₁₂ ClO ₇	291.02762	291.02771	-0.30
C ₁₁ H ₁₄ ClO ₇	293.04339	293.04336	0.11
C ₁₂ H ₄ ClO ₇	294.96532	294.96511	0.72
C ₁₂ H ₆ ClO ₇	296.98090	296.98076	0.48
C ₁₂ H ₈ ClO ₇	298.99646	298.99641	0.18
C ₁₂ H ₁₀ ClO ₇	301.01204	301.01206	-0.06
C ₁₂ H ₁₂ ClO ₇	303.02766	303.02771	-0.16
C ₁₂ H ₁₄ ClO ₇	305.04330	305.04336	-0.19
C ₁₂ H ₁₆ ClO ₇	307.05898	307.05901	-0.09
C ₁₃ H ₆ ClO ₇	308.98095	308.98076	0.62
C ₁₃ H ₈ ClO ₇	310.99659	310.99641	0.59
C ₁₃ H ₁₀ ClO ₇	313.01222	313.01206	0.52
C ₁₃ H ₁₄ ClO ₇	317.04324	317.04336	-0.37
C ₁₃ H ₁₆ ClO ₇	319.05883	319.05901	-0.55
C ₁₃ H ₁₈ ClO ₇	321.07449	321.07466	-0.52
C ₁₄ H ₈ ClO ₇	322.99667	322.99641	0.81
C ₁₄ H ₁₀ ClO ₇	325.01217	325.01206	0.35
C ₁₄ H ₁₂ ClO ₇	327.02755	327.02771	-0.48
C ₁₄ H ₁₄ ClO ₇	329.04321	329.04336	-0.45
C ₁₄ H ₁₆ ClO ₇	331.05910	331.05901	0.28
C ₁₄ H ₁₈ ClO ₇	333.07455	333.07466	-0.32
C ₁₄ H ₂₀ ClO ₇	335.09009	335.09031	-0.65
C ₁₄ H ₂₂ ClO ₇	337.10608	337.10596	0.36
C ₁₅ H ₁₂ ClO ₇	339.02758	339.02771	-0.37
C ₁₅ H ₁₄ ClO ₇	341.04334	341.04336	-0.05
C ₁₅ H ₁₆ ClO ₇	343.05904	343.05901	0.10
C ₁₅ H ₁₈ ClO ₇	345.07446	345.07466	-0.57
C ₁₅ H ₂₀ ClO ₇	347.09050	347.09031	0.56
C ₁₅ H ₂₂ ClO ₇	349.10575	349.10596	-0.59
C ₁₅ H ₂₄ ClO ₇	351.12179	351.12161	0.52
C ₁₆ H ₁₄ ClO ₇	353.04314	353.04336	-0.61
C ₁₆ H ₁₆ ClO ₇	355.05926	355.05901	0.71
C ₁₆ H ₁₈ ClO ₇	357.07448	357.07466	-0.50
C ₁₆ H ₂₀ ClO ₇	359.09045	359.09031	0.40

C ₁₆ H ₂₂ ClO ₇	361.10589	361.10596	-0.19
C ₁₆ H ₂₄ ClO ₇	363.12148	363.12161	-0.35
C ₁₆ H ₂₆ ClO ₇	365.13745	365.13726	0.53
C ₁₇ H ₁₆ ClO ₇	367.05878	367.05901	-0.62
C ₁₇ H ₁₈ ClO ₇	369.07470	369.07466	0.12
C ₁₇ H ₂₀ ClO ₇	371.09045	371.09031	0.39
C ₁₇ H ₂₂ ClO ₇	373.10573	373.10596	-0.61
C ₁₇ H ₂₄ ClO ₇	375.12169	375.12161	0.22
C ₁₇ H ₂₆ ClO ₇	377.13742	377.13726	0.43
C ₁₇ H ₂₈ ClO ₇	379.15264	379.15291	-0.70
C ₁₈ H ₁₈ ClO ₇	381.07454	381.07466	-0.31
C ₁₈ H ₂₀ ClO ₇	383.09056	383.09031	0.66
C ₁₈ H ₂₂ ClO ₇	385.10598	385.10596	0.06
C ₁₈ H ₂₄ ClO ₇	387.12137	387.12161	-0.61
C ₁₈ H ₂₆ ClO ₇	389.13713	389.13726	-0.33
C ₁₈ H ₂₈ ClO ₇	391.15304	391.15291	0.34
C ₁₈ H ₃₀ ClO ₇	393.16840	393.16856	-0.40
C ₁₉ H ₂₀ ClO ₇	395.09025	395.09031	-0.14
C ₁₉ H ₂₂ ClO ₇	397.10570	397.10596	-0.65
C ₁₉ H ₂₄ ClO ₇	399.12149	399.12161	-0.29
C ₁₉ H ₂₆ ClO ₇	401.13732	401.13726	0.16
C ₁₉ H ₂₈ ClO ₇	403.15319	403.15291	0.70
C ₁₉ H ₃₀ ClO ₇	405.16875	405.16856	0.48
C ₂₀ H ₂₂ ClO ₇	409.10592	409.10596	-0.09
C ₂₀ H ₂₄ ClO ₇	411.12141	411.12161	-0.48
C ₂₀ H ₂₆ ClO ₇	413.13701	413.13726	-0.60
C ₂₀ H ₂₈ ClO ₇	415.15273	415.15291	-0.43
C ₂₀ H ₃₀ ClO ₇	417.16847	417.16856	-0.21
C ₂₀ H ₃₂ ClO ₇	419.18399	419.18421	-0.52
C ₂₁ H ₂₄ ClO ₇	423.12170	423.12161	0.22
C ₂₁ H ₂₆ ClO ₇	425.13734	425.13726	0.20
C ₂₁ H ₂₈ ClO ₇	427.15324	427.15291	0.78
C ₂₁ H ₃₀ ClO ₇	429.16878	429.16856	0.52
C ₂₁ H ₃₂ ClO ₇	431.18435	431.18421	0.33
C ₂₁ H ₃₄ ClO ₇	433.20014	433.19986	0.65
C ₂₂ H ₂₆ ClO ₇	437.13746	437.13726	0.46
C ₂₂ H ₂₈ ClO ₇	439.15292	439.15291	0.03
C ₂₂ H ₃₀ ClO ₇	441.16854	441.16856	-0.04
C ₂₂ H ₃₂ ClO ₇	443.18404	443.18421	-0.38
C ₂₂ H ₃₄ ClO ₇	445.19950	445.19986	-0.80
C ₂₂ H ₃₆ ClO ₇	447.21515	447.21551	-0.80
C ₂₃ H ₂₈ ClO ₇	451.15282	451.15291	-0.19
C ₂₃ H ₃₀ ClO ₇	453.16868	453.16856	0.27
C ₂₃ H ₃₂ ClO ₇	455.18436	455.18421	0.34
C ₂₄ H ₃₀ ClO ₇	465.16851	465.16856	-0.10
C ₂₄ H ₃₂ ClO ₇	467.18431	467.18421	0.22
C ₂₄ H ₃₄ ClO ₇	469.20003	469.19986	0.37
C ₂₅ H ₃₀ ClO ₇	477.16857	477.16856	0.03

C ₉ H ₄ ClO ₈	274.96017	274.96002	0.54
C ₉ H ₆ ClO ₈	276.97558	276.97567	-0.33
C ₉ H ₈ ClO ₈	278.99147	278.99132	0.53
C ₁₀ H ₄ ClO ₈	286.96002	286.96002	0
C ₁₀ H ₆ ClO ₈	288.97556	288.97567	-0.39
C ₁₀ H ₈ ClO ₈	290.99120	290.99132	-0.42
C ₁₀ H ₁₀ ClO ₈	293.00696	293.00697	-0.04
C ₁₁ H ₆ ClO ₈	300.97570	300.97567	0.09
C ₁₁ H ₈ ClO ₈	302.99129	302.99132	-0.11
C ₁₁ H ₁₀ ClO ₈	305.00695	305.00697	-0.07
C ₁₁ H ₁₂ ClO ₈	307.02260	307.02262	-0.07
C ₁₂ H ₄ ClO ₈	310.96023	310.96002	0.67
C ₁₂ H ₆ ClO ₈	312.97586	312.97567	0.60
C ₁₂ H ₁₀ ClO ₈	317.00685	317.00697	-0.38
C ₁₂ H ₁₂ ClO ₈	319.02241	319.02262	-0.66
C ₁₂ H ₁₄ ClO ₈	321.03812	321.03827	-0.47
C ₁₃ H ₈ ClO ₈	326.99115	326.99132	-0.53
C ₁₃ H ₁₀ ClO ₈	329.00684	329.00697	-0.40
C ₁₃ H ₁₂ ClO ₈	331.02280	331.02262	0.54
C ₁₃ H ₁₄ ClO ₈	333.03813	333.03827	-0.43
C ₁₃ H ₁₆ ClO ₈	335.05372	335.05392	-0.60
C ₁₃ H ₁₈ ClO ₈	337.06971	337.06957	0.41
C ₁₄ H ₈ ClO ₈	338.99122	338.99132	-0.30
C ₁₄ H ₁₀ ClO ₈	341.00696	341.00697	-0.04
C ₁₄ H ₁₂ ClO ₈	343.02263	343.02262	0.02
C ₁₄ H ₁₄ ClO ₈	345.03810	345.03827	-0.50
C ₁₄ H ₁₆ ClO ₈	347.05410	347.05392	0.51
C ₁₄ H ₁₈ ClO ₈	349.06934	349.06957	-0.66
C ₁₄ H ₂₀ ClO ₈	351.08543	351.08522	0.59
C ₁₅ H ₁₀ ClO ₈	353.00678	353.00697	-0.54
C ₁₅ H ₁₂ ClO ₈	355.02285	355.02262	0.64
C ₁₅ H ₁₄ ClO ₈	357.03810	357.03827	-0.48
C ₁₅ H ₁₆ ClO ₈	359.05395	359.05392	0.08
C ₁₅ H ₁₈ ClO ₈	361.06945	361.06957	-0.34
C ₁₅ H ₂₀ ClO ₈	363.08504	363.08522	-0.50
C ₁₅ H ₂₂ ClO ₈	365.10109	365.10087	0.60
C ₁₆ H ₁₂ ClO ₈	367.02248	367.02262	-0.39
C ₁₆ H ₁₄ ClO ₈	369.03832	369.03827	0.13
C ₁₆ H ₁₆ ClO ₈	371.05404	371.05392	0.32
C ₁₆ H ₁₈ ClO ₈	373.06931	373.06957	-0.70
C ₁₆ H ₂₀ ClO ₈	375.08533	375.08522	0.29
C ₁₆ H ₂₂ ClO ₈	377.10097	377.10087	0.26
C ₁₆ H ₂₄ ClO ₈	379.11620	379.11652	-0.85
C ₁₇ H ₁₄ ClO ₈	381.03816	381.03827	-0.29
C ₁₇ H ₁₆ ClO ₈	383.05419	383.05392	0.70
C ₁₇ H ₁₈ ClO ₈	385.06957	385.06957	0
C ₁₇ H ₂₀ ClO ₈	387.08496	387.08522	-0.68
C ₁₇ H ₂₂ ClO ₈	389.10071	389.10087	-0.42

$C_{17}H_{24}ClO_8$	391.11672	391.11652	0.51
$C_{17}H_{26}ClO_8$	393.13221	393.13217	0.10
$C_{18}H_{16}ClO_8$	395.05390	395.05392	-0.06
$C_{18}H_{18}ClO_8$	397.06933	397.06957	-0.61
$C_{18}H_{20}ClO_8$	399.08501	399.08522	-0.53
$C_{18}H_{22}ClO_8$	401.10088	401.10087	0.02
$C_{18}H_{24}ClO_8$	403.11675	403.11652	0.57
$C_{18}H_{26}ClO_8$	405.13238	405.13217	0.51
$C_{19}H_{18}ClO_8$	409.06948	409.06957	-0.22
$C_{19}H_{20}ClO_8$	411.08505	411.08522	-0.42
$C_{19}H_{22}ClO_8$	413.10061	413.10087	-0.63
$C_{19}H_{24}ClO_8$	415.11629	415.11652	-0.56
$C_{19}H_{26}ClO_8$	417.13201	417.13217	-0.39
$C_{19}H_{28}ClO_8$	419.14763	419.14782	-0.46
$C_{19}H_{30}ClO_8$	421.16315	421.16347	-0.76
$C_{20}H_{20}ClO_8$	423.08511	423.08522	-0.26
$C_{20}H_{22}ClO_8$	425.10085	425.10087	-0.05
$C_{20}H_{24}ClO_8$	427.11662	427.11652	0.23
$C_{20}H_{26}ClO_8$	429.13225	429.13217	0.18
$C_{20}H_{28}ClO_8$	431.14791	431.14782	0.20
$C_{20}H_{30}ClO_8$	433.16351	433.16347	0.09
$C_{20}H_{32}ClO_8$	435.17906	435.17912	-0.14
$C_{21}H_{22}ClO_8$	437.10078	437.10087	-0.21
$C_{21}H_{24}ClO_8$	439.11660	439.11652	0.18
$C_{21}H_{26}ClO_8$	441.13214	441.13217	-0.07
$C_{21}H_{28}ClO_8$	443.14763	443.14782	-0.43
$C_{21}H_{30}ClO_8$	445.16329	445.16347	-0.41
$C_{21}H_{32}ClO_8$	447.17882	447.17912	-0.68
$C_{21}H_{34}ClO_8$	449.19455	449.19477	-0.49
$C_{22}H_{24}ClO_8$	451.11657	451.11652	0.11
$C_{22}H_{26}ClO_8$	453.13219	453.13217	0.04
$C_{22}H_{28}ClO_8$	455.14804	455.14782	0.48
$C_{22}H_{30}ClO_8$	457.16385	457.16347	0.83
$C_{22}H_{32}ClO_8$	459.17916	459.17912	0.08
$C_{22}H_{34}ClO_8$	461.19475	461.19477	-0.05
$C_{23}H_{26}ClO_8$	465.13206	465.13217	-0.24
$C_{23}H_{28}ClO_8$	467.14781	467.14782	-0.03
$C_{23}H_{30}ClO_8$	469.16344	469.16347	-0.07
$C_{23}H_{32}ClO_8$	471.17911	471.17912	-0.03
$C_{23}H_{34}ClO_8$	473.19493	473.19477	0.33
$C_{24}H_{26}ClO_8$	477.13236	477.13217	0.39
$C_{24}H_{28}ClO_8$	479.14802	479.14782	0.41
$C_{24}H_{30}ClO_8$	481.16365	481.16347	0.37
$C_{24}H_{32}ClO_8$	483.17948	483.17912	0.74
$C_{24}H_{34}ClO_8$	485.19463	485.19477	-0.29
$C_{10}H_6ClO_9$	304.97056	304.97059	-0.09
$C_{10}H_8ClO_9$	306.98625	306.98624	0.04
$C_{11}H_6ClO_9$	316.97044	316.97059	-0.46

C ₁₁ H ₈ ClO ₉	318.98603	318.98624	-0.65
C ₁₁ H ₁₀ ClO ₉	321.00177	321.00189	-0.36
C ₁₂ H ₈ ClO ₉	330.98644	330.98624	0.61
C ₁₂ H ₁₀ ClO ₉	333.00172	333.00189	-0.50
C ₁₂ H ₁₂ ClO ₉	335.01737	335.01754	-0.50
C ₁₂ H ₁₄ ClO ₉	337.03336	337.03319	0.51
C ₁₃ H ₈ ClO ₉	342.98627	342.98624	0.10
C ₁₃ H ₁₀ ClO ₉	345.00174	345.00189	-0.43
C ₁₃ H ₁₂ ClO ₉	347.01772	347.01754	0.53
C ₁₃ H ₁₄ ClO ₉	349.03297	349.03319	-0.62
C ₁₃ H ₁₆ ClO ₉	351.04899	351.04884	0.44
C ₁₄ H ₈ ClO ₉	354.98643	354.98624	0.54
C ₁₄ H ₁₀ ClO ₉	357.00176	357.00189	-0.36
C ₁₄ H ₁₂ ClO ₉	359.01754	359.01754	0
C ₁₄ H ₁₄ ClO ₉	361.03324	361.03319	0.15
C ₁₄ H ₁₆ ClO ₉	363.04866	363.04884	-0.49
C ₁₄ H ₁₈ ClO ₉	365.06471	365.06449	0.61
C ₁₅ H ₁₀ ClO ₉	369.00193	369.00189	0.12
C ₁₅ H ₁₂ ClO ₉	371.01776	371.01754	0.60
C ₁₅ H ₁₄ ClO ₉	373.03297	373.03319	-0.58
C ₁₅ H ₁₆ ClO ₉	375.04878	375.04884	-0.15
C ₁₅ H ₁₈ ClO ₉	377.06468	377.06449	0.51
C ₁₅ H ₂₀ ClO ₉	379.07986	379.08014	-0.73
C ₁₆ H ₁₀ ClO ₉	381.00182	381.00189	-0.18
C ₁₆ H ₁₂ ClO ₉	383.01781	383.01754	0.71
C ₁₆ H ₁₄ ClO ₉	385.03332	385.03319	0.35
C ₁₆ H ₁₆ ClO ₉	387.04860	387.04884	-0.61
C ₁₆ H ₁₈ ClO ₉	389.06430	389.06449	-0.48
C ₁₆ H ₂₀ ClO ₉	391.08037	391.08014	0.60
C ₁₆ H ₂₂ ClO ₉	393.09592	393.09579	0.34
C ₁₇ H ₁₂ ClO ₉	395.01756	395.01754	0.06
C ₁₇ H ₁₄ ClO ₉	397.03306	397.03319	-0.32
C ₁₇ H ₁₆ ClO ₉	399.04864	399.04884	-0.49
C ₁₇ H ₁₈ ClO ₉	401.06446	401.06449	-0.07
C ₁₇ H ₂₀ ClO ₉	403.08038	403.08014	0.60
C ₁₇ H ₂₂ ClO ₉	405.09601	405.09579	0.55
C ₁₇ H ₂₄ ClO ₉	407.11138	407.11144	-0.14
C ₁₈ H ₁₄ ClO ₉	409.03304	409.03319	-0.36
C ₁₈ H ₁₆ ClO ₉	411.04862	411.04884	-0.53
C ₁₈ H ₁₈ ClO ₉	413.06425	413.06449	-0.57
C ₁₈ H ₂₀ ClO ₉	415.07987	415.08014	-0.64
C ₁₈ H ₂₂ ClO ₉	417.09556	417.09579	-0.54
C ₁₈ H ₂₄ ClO ₉	419.11129	419.11144	-0.35
C ₁₉ H ₁₆ ClO ₉	423.04888	423.04884	0.10
C ₁₉ H ₁₈ ClO ₉	425.06450	425.06449	0.03
C ₁₉ H ₂₀ ClO ₉	427.08012	427.08014	-0.04
C ₁₉ H ₂₂ ClO ₉	429.09585	429.09579	0.15
C ₁₉ H ₂₄ ClO ₉	431.11151	431.11144	0.17

C ₁₉ H ₂₆ ClO ₉	433.12716	433.12709	0.17
C ₁₉ H ₂₈ ClO ₉	435.14263	435.14274	-0.25
C ₂₀ H ₁₈ ClO ₉	437.06427	437.06449	-0.50
C ₂₀ H ₂₀ ClO ₉	439.08009	439.08014	-0.11
C ₂₀ H ₂₂ ClO ₉	441.09557	441.09579	-0.49
C ₂₀ H ₂₄ ClO ₉	443.11122	443.11144	-0.49
C ₂₀ H ₂₆ ClO ₉	445.12688	445.12709	-0.47
C ₂₀ H ₂₈ ClO ₉	447.14239	447.14274	-0.78
C ₂₀ H ₃₀ ClO ₉	449.15806	449.15839	-0.73
C ₂₁ H ₂₀ ClO ₉	451.07997	451.08014	-0.37
C ₂₁ H ₂₂ ClO ₉	453.09568	453.09579	-0.24
C ₂₁ H ₂₄ ClO ₉	455.11159	455.11144	0.34
C ₂₁ H ₂₆ ClO ₉	457.12740	457.12709	0.68
C ₂₁ H ₂₈ ClO ₉	459.14284	459.14274	0.22
C ₂₁ H ₃₀ ClO ₉	461.15833	461.15839	-0.12
C ₂₁ H ₃₂ ClO ₉	463.17382	463.17404	-0.47
C ₂₂ H ₂₂ ClO ₉	465.09571	465.09579	-0.17
C ₂₂ H ₂₄ ClO ₉	467.11125	467.11144	-0.40
C ₂₂ H ₂₆ ClO ₉	469.12711	469.12709	0.05
C ₂₂ H ₂₈ ClO ₉	471.14279	471.14274	0.11
C ₂₂ H ₃₀ ClO ₉	473.15856	473.15839	0.37
C ₂₃ H ₂₂ ClO ₉	477.09548	477.09579	-0.64
C ₂₃ H ₂₄ ClO ₉	479.11178	479.11144	0.72
C ₂₃ H ₂₆ ClO ₉	481.12735	481.12709	0.55
C ₂₃ H ₂₈ ClO ₉	483.14318	483.14274	0.92
C ₂₃ H ₃₀ ClO ₉	485.15838	485.15839	-0.01
C ₂₃ H ₃₂ ClO ₉	487.17385	487.17404	-0.38
C ₁₁ H ₈ ClO ₁₀	334.98096	334.98115	-0.57
C ₁₁ H ₁₀ ClO ₁₀	336.99697	336.99680	0.50
C ₁₂ H ₈ ClO ₁₀	346.98121	346.98115	0.17
C ₁₂ H ₁₀ ClO ₁₀	348.99660	348.99680	-0.58
C ₁₂ H ₁₂ ClO ₁₀	351.01268	351.01245	0.65
C ₁₃ H ₁₀ ClO ₁₀	360.99678	360.99680	-0.06
C ₁₃ H ₁₂ ClO ₁₀	363.01230	363.01245	-0.42
C ₁₃ H ₁₄ ClO ₁₀	365.02834	365.02810	0.65
C ₁₄ H ₁₀ ClO ₁₀	372.99655	372.99680	-0.68
C ₁₄ H ₁₂ ClO ₁₀	375.01248	375.01245	0.07
C ₁₄ H ₁₄ ClO ₁₀	377.02827	377.02810	0.45
C ₁₄ H ₁₆ ClO ₁₀	379.04361	379.04375	-0.37
C ₁₅ H ₁₀ ClO ₁₀	384.99681	384.99680	0.02
C ₁₅ H ₁₂ ClO ₁₀	387.01225	387.01245	-0.52
C ₁₅ H ₁₄ ClO ₁₀	389.02792	389.02810	-0.47
C ₁₅ H ₁₆ ClO ₁₀	391.04388	391.04375	0.33
C ₁₅ H ₁₈ ClO ₁₀	393.05959	393.05940	0.48
C ₁₆ H ₁₀ ClO ₁₀	396.99666	396.99680	-0.36
C ₁₆ H ₁₂ ClO ₁₀	399.01228	399.01245	-0.43
C ₁₆ H ₁₄ ClO ₁₀	401.02810	401.02810	0
C ₁₆ H ₁₆ ClO ₁₀	403.04392	403.04375	0.42

C ₁₆ H ₁₈ ClO ₁₀	405.05968	405.05940	0.69
C ₁₆ H ₂₀ ClO ₁₀	407.07504	407.07505	-0.03
C ₁₇ H ₁₂ ClO ₁₀	411.01228	411.01245	-0.42
C ₁₇ H ₁₄ ClO ₁₀	413.02787	413.02810	-0.56
C ₁₇ H ₁₆ ClO ₁₀	415.04349	415.04375	-0.63
C ₁₇ H ₁₈ ClO ₁₀	417.05920	417.05940	-0.48
C ₁₇ H ₂₀ ClO ₁₀	419.07485	419.07505	-0.48
C ₁₇ H ₂₂ ClO ₁₀	421.09043	421.09070	-0.65
C ₁₈ H ₁₄ ClO ₁₀	425.02786	425.02810	-0.57
C ₁₈ H ₁₆ ClO ₁₀	427.04365	427.04375	-0.24
C ₁₈ H ₁₈ ClO ₁₀	429.05943	429.05940	0.07
C ₁₈ H ₂₀ ClO ₁₀	431.07500	431.07505	-0.12
C ₁₈ H ₂₂ ClO ₁₀	433.09063	433.09070	-0.17
C ₁₈ H ₂₄ ClO ₁₀	435.10599	435.10635	-0.83
C ₁₉ H ₁₄ ClO ₁₀	437.02799	437.02810	-0.26
C ₁₉ H ₁₆ ClO ₁₀	439.04367	439.04375	-0.19
C ₁₉ H ₁₈ ClO ₁₀	441.05934	441.05940	-0.14
C ₁₉ H ₂₀ ClO ₁₀	443.07487	443.07505	-0.41
C ₁₉ H ₂₂ ClO ₁₀	445.09042	445.09070	-0.63
C ₁₉ H ₂₄ ClO ₁₀	447.10606	447.10635	-0.65
C ₁₉ H ₂₆ ClO ₁₀	449.12176	449.12200	-0.54
C ₂₀ H ₁₆ ClO ₁₀	451.04392	451.04375	0.37
C ₂₀ H ₁₈ ClO ₁₀	453.05937	453.05940	-0.07
C ₂₀ H ₂₀ ClO ₁₀	455.07509	455.07505	0.08
C ₂₀ H ₂₂ ClO ₁₀	457.09087	457.09070	0.37
C ₂₀ H ₂₄ ClO ₁₀	459.10650	459.10635	0.32
C ₂₀ H ₂₆ ClO ₁₀	461.12183	461.12200	-0.37
C ₂₀ H ₂₈ ClO ₁₀	463.13740	463.13765	-0.54
C ₂₁ H ₁₈ ClO ₁₀	465.05896	465.05940	-0.95
C ₂₁ H ₂₀ ClO ₁₀	467.07497	467.07505	-0.18
C ₂₁ H ₂₂ ClO ₁₀	469.09070	469.09070	0.00
C ₂₁ H ₂₄ ClO ₁₀	471.10672	471.10635	0.78
C ₂₁ H ₂₆ ClO ₁₀	473.12222	473.12200	0.46
C ₂₁ H ₂₈ ClO ₁₀	475.13758	475.13765	-0.15
C ₂₂ H ₂₀ ClO ₁₀	479.07500	479.07505	-0.11
C ₂₂ H ₂₂ ClO ₁₀	481.09115	481.09070	0.93
C ₂₂ H ₂₄ ClO ₁₀	483.10666	483.10635	0.64
C ₂₂ H ₂₆ ClO ₁₀	485.12200	485.12200	0
C ₂₂ H ₂₈ ClO ₁₀	487.13736	487.13765	-0.60
C ₁₃ H ₁₂ ClO ₁₁	379.00717	379.00737	-0.52
C ₁₄ H ₁₀ ClO ₁₁	388.99153	388.99172	-0.48
C ₁₄ H ₁₂ ClO ₁₁	391.00750	391.00737	0.34
C ₁₄ H ₁₄ ClO ₁₁	393.02331	393.02302	0.75
C ₁₅ H ₁₂ ClO ₁₁	403.00763	403.00737	0.65
C ₁₅ H ₁₄ ClO ₁₁	405.02324	405.02302	0.55
C ₁₅ H ₁₆ ClO ₁₁	407.03884	407.03867	0.43
C ₁₆ H ₁₂ ClO ₁₁	415.00705	415.00737	-0.76
C ₁₆ H ₁₄ ClO ₁₁	417.02269	417.02302	-0.78

C ₁₆ H ₁₆ ClO ₁₁	419.03840	419.03867	-0.64
C ₁₆ H ₁₈ ClO ₁₁	421.05411	421.05432	-0.49
C ₁₇ H ₁₂ ClO ₁₁	427.00719	427.00737	-0.41
C ₁₇ H ₁₄ ClO ₁₁	429.02303	429.02302	0.03
C ₁₇ H ₁₆ ClO ₁₁	431.03864	431.03867	-0.06
C ₁₇ H ₁₈ ClO ₁₁	433.05427	433.05432	-0.11
C ₁₇ H ₂₀ ClO ₁₁	435.06980	435.06997	-0.38
C ₁₈ H ₁₄ ClO ₁₁	441.02292	441.02302	-0.22
C ₁₈ H ₁₆ ClO ₁₁	443.03842	443.03867	-0.56
C ₁₈ H ₁₈ ClO ₁₁	445.05409	445.05432	-0.51
C ₁₈ H ₂₀ ClO ₁₁	447.06967	447.06997	-0.66
C ₁₈ H ₂₂ ClO ₁₁	449.08533	449.08562	-0.64
C ₁₉ H ₁₆ ClO ₁₁	455.03885	455.03867	0.40
C ₁₉ H ₁₈ ClO ₁₁	457.05457	457.05432	0.55
C ₁₉ H ₂₀ ClO ₁₁	459.07016	459.06997	0.42
C ₁₉ H ₂₂ ClO ₁₁	461.08552	461.08562	-0.21
C ₁₉ H ₂₄ ClO ₁₁	463.10100	463.10127	-0.58
C ₂₀ H ₁₈ ClO ₁₁	469.05417	469.05432	-0.31
C ₂₀ H ₂₀ ClO ₁₁	471.07017	471.06997	0.43
C ₂₀ H ₂₂ ClO ₁₁	473.08562	473.08562	0
C ₂₀ H ₂₄ ClO ₁₁	475.10117	475.10127	-0.20
C ₂₁ H ₁₆ ClO ₁₁	479.03828	479.03867	-0.81
C ₂₁ H ₁₈ ClO ₁₁	481.05402	481.05432	-0.62
C ₂₁ H ₂₀ ClO ₁₁	483.07015	483.06997	0.38
C ₂₁ H ₂₂ ClO ₁₁	485.08556	485.08562	-0.12
C ₂₁ H ₂₄ ClO ₁₁	487.10104	487.10127	-0.47
C ₁₅ H ₁₂ ClO ₁₂	419.00204	419.00228	-0.58
C ₁₆ H ₁₆ ClO ₁₂	435.03349	435.03358	-0.21
C ₁₇ H ₁₄ ClO ₁₂	445.01774	445.01793	-0.43
C ₁₇ H ₁₆ ClO ₁₂	447.03327	447.03358	-0.70
C ₁₇ H ₁₈ ClO ₁₂	449.04898	449.04923	-0.56
C ₁₈ H ₁₄ ClO ₁₂	457.01788	457.01793	-0.11
C ₁₈ H ₁₆ ClO ₁₂	459.03357	459.03358	-0.03
C ₁₈ H ₁₈ ClO ₁₂	461.04913	461.04923	-0.22
C ₁₈ H ₂₀ ClO ₁₂	463.06466	463.06488	-0.48
C ₁₉ H ₁₆ ClO ₁₂	471.03348	471.03358	-0.22
C ₁₉ H ₁₈ ClO ₁₂	473.04921	473.04923	-0.05
C ₁₉ H ₂₀ ClO ₁₂	475.06486	475.06488	-0.05
C ₂₀ H ₂₀ ClO ₁₂	487.06477	487.06488	-0.23

two chlorine-containing products

formula (M-H) ⁻	measured mass	theoretical mass	error (ppm)
C ₆ H ₅ Cl ₂ O ₃	194.96220	194.96213	0.38
C ₆ H ₇ Cl ₂ O ₃	196.97785	196.97778	0.38
C ₇ H ₅ Cl ₂ O ₃	206.96212	206.96213	-0.02
C ₈ H ₇ Cl ₂ O ₃	220.97788	220.97778	0.48
C ₈ H ₉ Cl ₂ O ₃	222.99347	222.99343	0.20
C ₈ H ₁₁ Cl ₂ O ₃	225.00900	225.00908	-0.33

C ₉ H ₁₁ Cl ₂ O ₃	237.00909	237.00908	0.06
C ₉ H ₁₃ Cl ₂ O ₃	239.02459	239.02473	-0.56
C ₁₀ H ₇ Cl ₂ O ₃	244.97787	244.97778	0.39
C ₁₀ H ₁₁ Cl ₂ O ₃	249.00917	249.00908	0.38
C ₁₀ H ₁₃ Cl ₂ O ₃	251.02484	251.02473	0.46
C ₁₀ H ₁₅ Cl ₂ O ₃	253.04044	253.04038	0.26
C ₁₁ H ₉ Cl ₂ O ₃	258.99342	258.99343	-0.02
C ₁₁ H ₁₁ Cl ₂ O ₃	261.00917	261.00908	0.36
C ₁₁ H ₁₇ Cl ₂ O ₃	267.05599	267.05603	-0.13
C ₁₂ H ₁₁ Cl ₂ O ₃	273.00913	273.00908	0.20
C ₁₂ H ₁₃ Cl ₂ O ₃	275.02491	275.02473	0.67
C ₁₂ H ₁₅ Cl ₂ O ₃	277.04019	277.04038	-0.67
C ₁₄ H ₁₉ Cl ₂ O ₃	305.07150	305.07168	-0.57
C ₆ H ₃ Cl ₂ O ₄	208.94150	208.94139	0.53
C ₆ H ₅ Cl ₂ O ₄	210.95709	210.95704	0.24
C ₆ H ₇ Cl ₂ O ₄	212.97268	212.97269	-0.05
C ₇ H ₅ Cl ₂ O ₄	222.95702	222.95704	-0.09
C ₇ H ₇ Cl ₂ O ₄	224.97265	224.97269	-0.18
C ₇ H ₉ Cl ₂ O ₄	226.98843	226.98834	0.40
C ₈ H ₇ Cl ₂ O ₄	236.97273	236.97269	0.17
C ₈ H ₉ Cl ₂ O ₄	238.98830	238.98834	-0.17
C ₈ H ₁₁ Cl ₂ O ₄	241.00404	241.00399	0.21
C ₉ H ₇ Cl ₂ O ₄	248.97282	248.97269	0.52
C ₉ H ₉ Cl ₂ O ₄	250.98847	250.98834	0.52
C ₉ H ₁₁ Cl ₂ O ₄	253.00414	253.00399	0.59
C ₉ H ₁₃ Cl ₂ O ₄	255.01973	255.01964	0.35
C ₁₀ H ₅ Cl ₂ O ₄	258.95700	258.95704	-0.15
C ₁₀ H ₇ Cl ₂ O ₄	260.97280	260.97269	0.42
C ₁₀ H ₉ Cl ₂ O ₄	262.98839	262.98834	0.19
C ₁₀ H ₁₁ Cl ₂ O ₄	265.00391	265.00399	-0.30
C ₁₀ H ₁₃ Cl ₂ O ₄	267.01963	267.01964	-0.04
C ₁₀ H ₁₅ Cl ₂ O ₄	269.03525	269.03529	-0.15
C ₁₁ H ₇ Cl ₂ O ₄	272.97261	272.97269	-0.29
C ₁₁ H ₉ Cl ₂ O ₄	274.98842	274.98834	0.29
C ₁₁ H ₁₁ Cl ₂ O ₄	277.00387	277.00399	-0.43
C ₁₁ H ₁₃ Cl ₂ O ₄	279.01978	279.01964	0.50
C ₁₁ H ₁₅ Cl ₂ O ₄	281.03520	281.03529	-0.32
C ₁₁ H ₁₇ Cl ₂ O ₄	283.05079	283.05094	-0.53
C ₁₂ H ₉ Cl ₂ O ₄	286.98833	286.98834	-0.03
C ₁₂ H ₁₁ Cl ₂ O ₄	289.00384	289.00399	-0.52
C ₁₂ H ₁₃ Cl ₂ O ₄	291.01952	291.01964	-0.41
C ₁₂ H ₁₅ Cl ₂ O ₄	293.03532	293.03529	0.10
C ₁₂ H ₁₇ Cl ₂ O ₄	295.05107	295.05094	0.44
C ₁₂ H ₁₉ Cl ₂ O ₄	297.06668	297.06659	0.30
C ₁₃ H ₁₁ Cl ₂ O ₄	301.00395	301.00399	-0.13
C ₁₃ H ₁₃ Cl ₂ O ₄	303.01958	303.01964	-0.20
C ₁₃ H ₁₅ Cl ₂ O ₄	305.03519	305.03529	-0.33
C ₁₃ H ₁₇ Cl ₂ O ₄	307.05090	307.05094	-0.13

C ₁₃ H ₁₉ Cl ₂ O ₄	309.06655	309.06659	-0.13
C ₁₄ H ₁₅ Cl ₂ O ₄	317.03515	317.03529	-0.44
C ₁₄ H ₁₇ Cl ₂ O ₄	319.05070	319.05094	-0.75
C ₁₄ H ₁₉ Cl ₂ O ₄	321.06636	321.06659	-0.72
C ₁₄ H ₂₁ Cl ₂ O ₄	323.08216	323.08224	-0.25
C ₁₅ H ₂₃ Cl ₂ O ₄	337.09798	337.09789	0.27
C ₆ H ₃ Cl ₂ O ₅	224.93627	224.93631	-0.16
C ₆ H ₅ Cl ₂ O ₅	226.95204	226.95196	0.37
C ₇ H ₃ Cl ₂ O ₅	236.93638	236.93631	0.32
C ₇ H ₅ Cl ₂ O ₅	238.95192	238.95196	-0.15
C ₇ H ₇ Cl ₂ O ₅	240.96756	240.96761	-0.19
C ₇ H ₉ Cl ₂ O ₅	242.98338	242.98326	0.51
C ₈ H ₃ Cl ₂ O ₅	248.93649	248.93631	0.74
C ₈ H ₅ Cl ₂ O ₅	250.95211	250.95196	0.62
C ₈ H ₇ Cl ₂ O ₅	252.96770	252.96761	0.38
C ₈ H ₉ Cl ₂ O ₅	254.98325	254.98326	-0.02
C ₈ H ₁₁ Cl ₂ O ₅	256.99884	256.99891	-0.25
C ₉ H ₃ Cl ₂ O ₅	260.93646	260.93631	0.59
C ₉ H ₅ Cl ₂ O ₅	262.95196	262.95196	0.02
C ₉ H ₇ Cl ₂ O ₅	264.96751	264.96761	-0.36
C ₉ H ₉ Cl ₂ O ₅	266.98335	266.98326	0.36
C ₉ H ₁₁ Cl ₂ O ₅	268.99883	268.99891	-0.28
C ₉ H ₁₃ Cl ₂ O ₅	271.01452	271.01456	-0.13
C ₁₀ H ₃ Cl ₂ O ₅	272.93627	272.93631	-0.13
C ₁₀ H ₅ Cl ₂ O ₅	274.95205	274.95196	0.35
C ₁₀ H ₇ Cl ₂ O ₅	276.96749	276.96761	-0.42
C ₁₀ H ₉ Cl ₂ O ₅	278.98340	278.98326	0.52
C ₁₀ H ₁₁ Cl ₂ O ₅	280.99881	280.99891	-0.34
C ₁₀ H ₁₃ Cl ₂ O ₅	283.01448	283.01456	-0.27
C ₁₀ H ₁₅ Cl ₂ O ₅	285.03039	285.03021	0.65
C ₁₁ H ₅ Cl ₂ O ₅	286.95205	286.95196	0.33
C ₁₁ H ₇ Cl ₂ O ₅	288.96746	288.96761	-0.50
C ₁₁ H ₁₁ Cl ₂ O ₅	292.99886	292.99891	-0.15
C ₁₁ H ₁₃ Cl ₂ O ₅	295.01468	295.01456	0.42
C ₁₁ H ₁₅ Cl ₂ O ₅	297.03030	297.03021	0.32
C ₁₁ H ₁₇ Cl ₂ O ₅	299.04592	299.04586	0.22
C ₁₂ H ₇ Cl ₂ O ₅	300.96762	300.96761	0.05
C ₁₂ H ₉ Cl ₂ O ₅	302.98328	302.98326	0.08
C ₁₂ H ₁₁ Cl ₂ O ₅	304.99888	304.99891	-0.08
C ₁₂ H ₁₃ Cl ₂ O ₅	307.01456	307.01456	0
C ₁₂ H ₁₅ Cl ₂ O ₅	309.03024	309.03021	0.11
C ₁₂ H ₁₇ Cl ₂ O ₅	311.04597	311.04586	0.37
C ₁₃ H ₁₁ Cl ₂ O ₅	316.99872	316.99891	-0.58
C ₁₃ H ₁₃ Cl ₂ O ₅	319.01432	319.01456	-0.74
C ₁₃ H ₁₅ Cl ₂ O ₅	321.03004	321.03021	-0.51
C ₁₃ H ₁₇ Cl ₂ O ₅	323.04590	323.04586	0.14
C ₁₃ H ₁₉ Cl ₂ O ₅	325.06160	325.06151	0.29
C ₁₄ H ₁₁ Cl ₂ O ₅	328.99875	328.99891	-0.47

C ₁₄ H ₁₃ Cl ₂ O ₅	331.01472	331.01456	0.50
C ₁₄ H ₁₅ Cl ₂ O ₅	333.03003	333.03021	-0.53
C ₁₄ H ₁₇ Cl ₂ O ₅	335.04562	335.04586	-0.70
C ₁₄ H ₁₉ Cl ₂ O ₅	337.06171	337.06151	0.61
C ₁₄ H ₂₁ Cl ₂ O ₅	339.07696	339.07716	-0.58
C ₁₅ H ₁₅ Cl ₂ O ₅	345.02999	345.03021	-0.62
C ₁₅ H ₁₇ Cl ₂ O ₅	347.04597	347.04586	0.33
C ₁₅ H ₁₉ Cl ₂ O ₅	349.06119	349.06151	-0.90
C ₁₅ H ₂₁ Cl ₂ O ₅	351.07732	351.07716	0.47
C ₁₅ H ₂₃ Cl ₂ O ₅	353.09253	353.09281	-0.78
C ₇ H ₅ Cl ₂ O ₆	254.94687	254.94687	0
C ₇ H ₇ Cl ₂ O ₆	256.96245	256.96252	-0.27
C ₈ H ₃ Cl ₂ O ₆	264.93115	264.93122	-0.26
C ₈ H ₅ Cl ₂ O ₆	266.94698	266.94687	0.41
C ₈ H ₇ Cl ₂ O ₆	268.96244	268.96252	-0.30
C ₈ H ₉ Cl ₂ O ₆	270.97821	270.97817	0.15
C ₉ H ₅ Cl ₂ O ₆	278.94699	278.94687	0.43
C ₉ H ₇ Cl ₂ O ₆	280.96247	280.96252	-0.18
C ₉ H ₉ Cl ₂ O ₆	282.97807	282.97817	-0.35
C ₉ H ₁₁ Cl ₂ O ₆	284.99398	284.99382	0.56
C ₁₀ H ₅ Cl ₂ O ₆	290.94673	290.94687	-0.48
C ₁₀ H ₇ Cl ₂ O ₆	292.96245	292.96252	-0.24
C ₁₀ H ₉ Cl ₂ O ₆	294.97828	294.97817	0.37
C ₁₀ H ₁₁ Cl ₂ O ₆	296.99394	296.99382	0.40
C ₁₀ H ₁₃ Cl ₂ O ₆	299.00954	299.00947	0.23
C ₁₁ H ₅ Cl ₂ O ₆	302.94688	302.94687	0.03
C ₁₁ H ₇ Cl ₂ O ₆	304.96250	304.96252	-0.07
C ₁₁ H ₉ Cl ₂ O ₆	306.97819	306.97817	0.07
C ₁₁ H ₁₁ Cl ₂ O ₆	308.99390	308.99382	0.26
C ₁₁ H ₁₃ Cl ₂ O ₆	311.00956	311.00947	0.29
C ₁₁ H ₁₅ Cl ₂ O ₆	313.02523	313.02512	0.35
C ₁₂ H ₇ Cl ₂ O ₆	316.96235	316.96252	-0.54
C ₁₂ H ₉ Cl ₂ O ₆	318.97797	318.97817	-0.63
C ₁₂ H ₁₁ Cl ₂ O ₆	320.99369	320.99382	-0.40
C ₁₂ H ₁₃ Cl ₂ O ₆	323.00960	323.00947	0.40
C ₁₂ H ₁₅ Cl ₂ O ₆	325.02520	325.02512	0.25
C ₁₂ H ₁₇ Cl ₂ O ₆	327.04057	327.04077	-0.61
C ₁₃ H ₇ Cl ₂ O ₆	328.96250	328.96252	-0.06
C ₁₃ H ₉ Cl ₂ O ₆	330.97841	330.97817	0.73
C ₁₃ H ₁₁ Cl ₂ O ₆	332.99367	332.99382	-0.45
C ₁₃ H ₁₃ Cl ₂ O ₆	335.00935	335.00947	-0.36
C ₁₃ H ₁₅ Cl ₂ O ₆	337.02530	337.02512	0.53
C ₁₃ H ₁₇ Cl ₂ O ₆	339.04065	339.04077	-0.35
C ₁₃ H ₁₉ Cl ₂ O ₆	341.05629	341.05642	-0.38
C ₁₄ H ₁₁ Cl ₂ O ₆	344.99374	344.99382	-0.23
C ₁₄ H ₁₃ Cl ₂ O ₆	347.00968	347.00947	0.61
C ₁₄ H ₁₅ Cl ₂ O ₆	349.02490	349.02512	-0.63
C ₁₄ H ₁₇ Cl ₂ O ₆	351.04100	351.04077	0.66

C ₁₄ H ₁₉ Cl ₂ O ₆	353.05617	353.05642	-0.71
C ₁₄ H ₂₁ Cl ₂ O ₆	355.07233	355.07207	0.73
C ₁₅ H ₁₃ Cl ₂ O ₆	359.00950	359.00947	0.08
C ₁₅ H ₁₅ Cl ₂ O ₆	361.02524	361.02512	0.33
C ₁₅ H ₁₉ Cl ₂ O ₆	365.05676	365.05642	0.93
C ₁₅ H ₂₁ Cl ₂ O ₆	367.07179	367.07207	-0.76
C ₁₆ H ₁₅ Cl ₂ O ₆	373.02490	373.02512	-0.59
C ₁₆ H ₁₇ Cl ₂ O ₆	375.04064	375.04077	-0.35
C ₁₆ H ₁₉ Cl ₂ O ₆	377.05664	377.05642	0.58
C ₁₆ H ₂₁ Cl ₂ O ₆	379.07191	379.07207	-0.42
C ₈ H ₃ Cl ₂ O ₇	280.92611	280.92614	-0.09
C ₈ H ₅ Cl ₂ O ₇	282.94167	282.94179	-0.41
C ₈ H ₇ Cl ₂ O ₇	284.95759	284.95744	0.54
C ₉ H ₃ Cl ₂ O ₇	292.92610	292.92614	-0.12
C ₉ H ₅ Cl ₂ O ₇	294.94189	294.94179	0.36
C ₉ H ₇ Cl ₂ O ₇	296.95755	296.95744	0.39
C ₉ H ₉ Cl ₂ O ₇	298.97313	298.97309	0.15
C ₁₀ H ₅ Cl ₂ O ₇	306.94179	306.94179	0
C ₁₀ H ₇ Cl ₂ O ₇	308.95752	308.95744	0.28
C ₁₀ H ₉ Cl ₂ O ₇	310.97320	310.97309	0.37
C ₁₀ H ₁₁ Cl ₂ O ₇	312.98887	312.98874	0.43
C ₁₀ H ₁₃ Cl ₂ O ₇	315.00433	315.00439	-0.17
C ₁₁ H ₅ Cl ₂ O ₇	318.94157	318.94179	-0.67
C ₁₁ H ₇ Cl ₂ O ₇	320.95735	320.95744	-0.26
C ₁₁ H ₉ Cl ₂ O ₇	322.97322	322.97309	0.42
C ₁₁ H ₁₁ Cl ₂ O ₇	324.98877	324.98874	0.11
C ₁₁ H ₁₃ Cl ₂ O ₇	327.00419	327.00439	-0.60
C ₁₂ H ₅ Cl ₂ O ₇	330.94198	330.94179	0.59
C ₁₂ H ₇ Cl ₂ O ₇	332.95733	332.95744	-0.32
C ₁₂ H ₉ Cl ₂ O ₇	334.97299	334.97309	-0.28
C ₁₂ H ₁₁ Cl ₂ O ₇	336.98892	336.98874	0.55
C ₁₂ H ₁₃ Cl ₂ O ₇	339.00421	339.00439	-0.52
C ₁₂ H ₁₅ Cl ₂ O ₇	341.02005	341.02004	0.04
C ₁₂ H ₁₇ Cl ₂ O ₇	343.03579	343.03569	0.31
C ₁₃ H ₇ Cl ₂ O ₇	344.95751	344.95744	0.22
C ₁₃ H ₉ Cl ₂ O ₇	346.97324	346.97309	0.45
C ₁₃ H ₁₁ Cl ₂ O ₇	348.98858	348.98874	-0.44
C ₁₃ H ₁₃ Cl ₂ O ₇	351.00462	351.00439	0.67
C ₁₃ H ₁₅ Cl ₂ O ₇	353.01984	353.02004	-0.55
C ₁₃ H ₁₇ Cl ₂ O ₇	355.03586	355.03569	0.49
C ₁₃ H ₁₉ Cl ₂ O ₇	357.05125	357.05134	-0.24
C ₁₄ H ₉ Cl ₂ O ₇	358.97308	358.97309	-0.01
C ₁₄ H ₁₁ Cl ₂ O ₇	360.98884	360.98874	0.29
C ₁₄ H ₁₃ Cl ₂ O ₇	363.00425	363.00439	-0.37
C ₁₄ H ₁₅ Cl ₂ O ₇	365.02027	365.02004	0.64
C ₁₄ H ₁₇ Cl ₂ O ₇	367.03552	367.03569	-0.45
C ₁₄ H ₁₉ Cl ₂ O ₇	369.05141	369.05134	0.20
C ₁₅ H ₁₁ Cl ₂ O ₇	372.98859	372.98874	-0.39

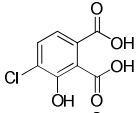
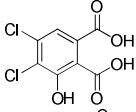
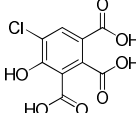
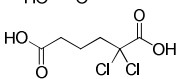
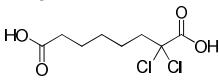
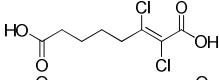
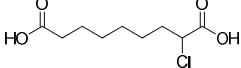
C ₁₅ H ₁₃ Cl ₂ O ₇	375.00441	375.00439	0.07
C ₁₅ H ₁₅ Cl ₂ O ₇	377.02026	377.02004	0.60
C ₁₅ H ₁₇ Cl ₂ O ₇	379.03553	379.03569	-0.41
C ₁₅ H ₁₉ Cl ₂ O ₇	381.05125	381.05134	-0.22
C ₁₅ H ₂₁ Cl ₂ O ₇	383.06725	383.06699	0.69
C ₁₆ H ₁₅ Cl ₂ O ₇	389.01988	389.02004	-0.40
C ₁₆ H ₁₇ Cl ₂ O ₇	391.03586	391.03569	0.45
C ₁₆ H ₁₉ Cl ₂ O ₇	393.05160	393.05134	0.67
C ₁₇ H ₁₅ Cl ₂ O ₇	401.01976	401.02004	-0.69
C ₁₇ H ₁₇ Cl ₂ O ₇	403.03590	403.03569	0.53
C ₁₇ H ₁₉ Cl ₂ O ₇	405.05154	405.05134	0.51
C ₁₈ H ₁₉ Cl ₂ O ₇	417.05110	417.05134	-0.56
C ₉ H ₃ Cl ₂ O ₈	308.92122	308.92105	0.55
C ₉ H ₅ Cl ₂ O ₈	310.93687	310.93670	0.55
C ₉ H ₇ Cl ₂ O ₈	312.95247	312.95235	0.38
C ₉ H ₉ Cl ₂ O ₈	314.96790	314.96800	-0.32
C ₁₀ H ₅ Cl ₂ O ₈	322.93690	322.93670	0.62
C ₁₀ H ₇ Cl ₂ O ₈	324.95238	324.95235	0.09
C ₁₀ H ₉ Cl ₂ O ₈	326.96779	326.96800	-0.64
C ₁₁ H ₇ Cl ₂ O ₈	336.95258	336.95235	0.68
C ₁₁ H ₉ Cl ₂ O ₈	338.96783	338.96800	-0.50
C ₁₁ H ₁₁ Cl ₂ O ₈	340.98378	340.98365	0.38
C ₁₁ H ₁₃ Cl ₂ O ₈	342.99928	342.99930	-0.06
C ₁₂ H ₅ Cl ₂ O ₈	346.93678	346.93670	0.23
C ₁₂ H ₉ Cl ₂ O ₈	350.96825	350.96800	0.71
C ₁₂ H ₁₁ Cl ₂ O ₈	352.98350	352.98365	-0.42
C ₁₂ H ₁₃ Cl ₂ O ₈	354.99952	354.99930	0.62
C ₁₂ H ₁₅ Cl ₂ O ₈	357.01492	357.01495	-0.08
C ₁₃ H ₇ Cl ₂ O ₈	360.95255	360.95235	0.55
C ₁₃ H ₉ Cl ₂ O ₈	362.96792	362.96800	-0.22
C ₁₃ H ₁₁ Cl ₂ O ₈	364.98398	364.98365	0.90
C ₁₃ H ₁₃ Cl ₂ O ₈	366.99913	366.99930	-0.46
C ₁₃ H ₁₅ Cl ₂ O ₈	369.01495	369.01495	0
C ₁₄ H ₇ Cl ₂ O ₈	372.95237	372.95235	0.05
C ₁₄ H ₉ Cl ₂ O ₈	374.96796	374.96800	-0.11
C ₁₄ H ₁₁ Cl ₂ O ₈	376.98397	376.98365	0.85
C ₁₄ H ₁₃ Cl ₂ O ₈	378.99920	378.99930	-0.26
C ₁₄ H ₁₅ Cl ₂ O ₈	381.01485	381.01495	-0.26
C ₁₄ H ₁₇ Cl ₂ O ₈	383.03091	383.03060	0.81
C ₁₅ H ₁₁ Cl ₂ O ₈	388.98352	388.98365	-0.33
C ₁₅ H ₁₃ Cl ₂ O ₈	390.99953	390.99930	0.59
C ₁₅ H ₁₅ Cl ₂ O ₈	393.01527	393.01495	0.81
C ₁₅ H ₁₇ Cl ₂ O ₈	395.03057	395.03060	-0.08
C ₁₅ H ₁₉ Cl ₂ O ₈	397.04612	397.04625	-0.33
C ₁₆ H ₁₁ Cl ₂ O ₈	400.98356	400.98365	-0.22
C ₁₆ H ₁₃ Cl ₂ O ₈	402.99953	402.99930	0.57
C ₁₆ H ₁₅ Cl ₂ O ₈	405.01517	405.01495	0.54
C ₁₆ H ₁₇ Cl ₂ O ₈	407.03075	407.03060	0.37

C ₁₆ H ₁₉ Cl ₂ O ₈	409.04624	409.04625	-0.02
C ₁₇ H ₁₅ Cl ₂ O ₈	417.01471	417.01495	-0.58
C ₁₇ H ₁₇ Cl ₂ O ₈	419.03032	419.03060	-0.67
C ₁₇ H ₁₉ Cl ₂ O ₈	421.04615	421.04625	-0.24
C ₁₈ H ₁₇ Cl ₂ O ₈	431.03061	431.03060	0.02
C ₁₈ H ₁₉ Cl ₂ O ₈	433.04608	433.04625	-0.39
C ₁₈ H ₂₁ Cl ₂ O ₈	435.06178	435.06190	-0.28
C ₁₉ H ₁₉ Cl ₂ O ₈	445.04607	445.04625	-0.40
C ₁₉ H ₂₁ Cl ₂ O ₈	447.06173	447.06190	-0.38
C ₁₀ H ₇ Cl ₂ O ₉	340.94747	340.94727	0.60
C ₁₀ H ₉ Cl ₂ O ₉	342.96305	342.96292	0.39
C ₁₁ H ₇ Cl ₂ O ₉	352.94719	352.94727	-0.21
C ₁₁ H ₉ Cl ₂ O ₉	354.96311	354.96292	0.55
C ₁₁ H ₁₁ Cl ₂ O ₉	356.97852	356.97857	-0.13
C ₁₂ H ₅ Cl ₂ O ₉	362.93140	362.93162	-0.59
C ₁₂ H ₉ Cl ₂ O ₉	366.96285	366.96292	-0.18
C ₁₂ H ₁₁ Cl ₂ O ₉	368.97860	368.97857	0.09
C ₁₂ H ₁₃ Cl ₂ O ₉	370.99453	370.99422	0.85
C ₁₃ H ₇ Cl ₂ O ₉	376.94758	376.94727	0.84
C ₁₃ H ₉ Cl ₂ O ₉	378.96285	378.96292	-0.17
C ₁₃ H ₁₁ Cl ₂ O ₉	380.97842	380.97857	-0.38
C ₁₃ H ₁₃ Cl ₂ O ₉	382.99453	382.99422	0.82
C ₁₃ H ₁₅ Cl ₂ O ₉	385.01021	385.00987	0.90
C ₁₄ H ₉ Cl ₂ O ₉	390.96308	390.96292	0.42
C ₁₄ H ₁₁ Cl ₂ O ₉	392.97886	392.97857	0.75
C ₁₄ H ₁₃ Cl ₂ O ₉	394.99435	394.99422	0.34
C ₁₄ H ₁₅ Cl ₂ O ₉	397.00976	397.00987	-0.26
C ₁₅ H ₁₁ Cl ₂ O ₉	404.97890	404.97857	0.83
C ₁₅ H ₁₃ Cl ₂ O ₉	406.99438	406.99422	0.41
C ₁₅ H ₁₅ Cl ₂ O ₉	409.00997	409.00987	0.26
C ₁₅ H ₁₇ Cl ₂ O ₉	411.02542	411.02552	-0.23
C ₁₅ H ₁₉ Cl ₂ O ₉	413.04117	413.04117	0.01
C ₁₆ H ₁₁ Cl ₂ O ₉	416.97835	416.97857	-0.52
C ₁₆ H ₁₃ Cl ₂ O ₉	418.99407	418.99422	-0.35
C ₁₆ H ₁₅ Cl ₂ O ₉	421.00992	421.00987	0.13
C ₁₆ H ₁₇ Cl ₂ O ₉	423.02555	423.02552	0.08
C ₁₆ H ₁₉ Cl ₂ O ₉	425.04120	425.04117	0.08
C ₁₇ H ₁₃ Cl ₂ O ₉	430.99424	430.99422	0.06
C ₁₇ H ₁₅ Cl ₂ O ₉	433.01001	433.00987	0.33
C ₁₇ H ₁₇ Cl ₂ O ₉	435.02558	435.02552	0.15
C ₁₇ H ₁₉ Cl ₂ O ₉	437.04113	437.04117	-0.08
C ₁₇ H ₂₁ Cl ₂ O ₉	439.05698	439.05682	0.38
C ₁₈ H ₁₅ Cl ₂ O ₉	445.00959	445.00987	-0.62
C ₁₈ H ₁₇ Cl ₂ O ₉	447.02534	447.02552	-0.39
C ₁₈ H ₁₉ Cl ₂ O ₉	449.04094	449.04117	-0.50
C ₁₈ H ₂₁ Cl ₂ O ₉	451.05679	451.05682	-0.06
C ₁₉ H ₁₉ Cl ₂ O ₉	461.04115	461.04117	-0.03
C ₂₀ H ₂₁ Cl ₂ O ₉	475.05673	475.05682	-0.18

C ₂₀ H ₂₃ Cl ₂ O ₉	477.07246	477.07247	-0.01
C ₁₁ H ₉ Cl ₂ O ₁₀	370.95816	370.95783	0.89
C ₁₂ H ₉ Cl ₂ O ₁₀	382.95803	382.95783	0.52
C ₁₂ H ₁₁ Cl ₂ O ₁₀	384.97370	384.97348	0.57
C ₁₂ H ₁₃ Cl ₂ O ₁₀	386.98913	386.98913	0
C ₁₃ H ₉ Cl ₂ O ₁₀	394.95803	394.95783	0.51
C ₁₃ H ₁₁ Cl ₂ O ₁₀	396.97336	396.97348	-0.30
C ₁₃ H ₁₃ Cl ₂ O ₁₀	398.98906	398.98913	-0.18
C ₁₄ H ₉ Cl ₂ O ₁₀	406.95812	406.95783	0.71
C ₁₄ H ₁₁ Cl ₂ O ₁₀	408.97353	408.97348	0.12
C ₁₄ H ₁₃ Cl ₂ O ₁₀	410.98901	410.98913	-0.29
C ₁₄ H ₁₅ Cl ₂ O ₁₀	413.00464	413.00478	-0.34
C ₁₄ H ₁₇ Cl ₂ O ₁₀	415.02046	415.02043	0.07
C ₁₅ H ₉ Cl ₂ O ₁₀	418.95765	418.95783	-0.43
C ₁₅ H ₁₁ Cl ₂ O ₁₀	420.97343	420.97348	-0.12
C ₁₅ H ₁₃ Cl ₂ O ₁₀	422.98917	422.98913	0.09
C ₁₅ H ₁₅ Cl ₂ O ₁₀	425.00481	425.00478	0.07
C ₁₅ H ₁₇ Cl ₂ O ₁₀	427.02072	427.02043	0.68
C ₁₆ H ₁₃ Cl ₂ O ₁₀	434.98902	434.98913	-0.25
C ₁₆ H ₁₅ Cl ₂ O ₁₀	437.00469	437.00478	-0.21
C ₁₆ H ₁₇ Cl ₂ O ₁₀	439.02033	439.02043	-0.23
C ₁₆ H ₁₉ Cl ₂ O ₁₀	441.03629	441.03608	0.48
C ₁₇ H ₁₁ Cl ₂ O ₁₀	444.97331	444.97348	-0.38
C ₁₇ H ₁₃ Cl ₂ O ₁₀	446.98910	446.98913	-0.07
C ₁₇ H ₁₅ Cl ₂ O ₁₀	449.00460	449.00478	-0.40
C ₁₇ H ₁₇ Cl ₂ O ₁₀	451.02046	451.02043	0.07
C ₁₇ H ₁₉ Cl ₂ O ₁₀	453.03632	453.03608	0.53
C ₁₈ H ₁₅ Cl ₂ O ₁₀	461.00489	461.00478	0.24
C ₁₈ H ₁₇ Cl ₂ O ₁₀	463.02024	463.02043	-0.41
C ₁₈ H ₁₉ Cl ₂ O ₁₀	465.03598	465.03608	-0.22
C ₁₈ H ₂₁ Cl ₂ O ₁₀	467.05196	467.05173	0.49
C ₁₉ H ₁₇ Cl ₂ O ₁₀	475.02031	475.02043	-0.25
C ₁₉ H ₁₉ Cl ₂ O ₁₀	477.03598	477.03608	-0.21
C ₁₉ H ₂₁ Cl ₂ O ₁₀	479.05179	479.05173	0.13
C ₁₂ H ₉ Cl ₂ O ₁₁	398.95272	398.95275	-0.06
C ₁₃ H ₉ Cl ₂ O ₁₁	410.95278	410.95275	0.09
C ₁₃ H ₁₁ Cl ₂ O ₁₁	412.96836	412.96840	-0.08
C ₁₃ H ₁₃ Cl ₂ O ₁₁	414.98402	414.98405	-0.06
C ₁₄ H ₉ Cl ₂ O ₁₁	422.95304	422.95275	0.70
C ₁₄ H ₁₁ Cl ₂ O ₁₁	424.96820	424.96840	-0.46
C ₁₄ H ₁₃ Cl ₂ O ₁₁	426.98406	426.98405	0.04
C ₁₄ H ₁₅ Cl ₂ O ₁₁	428.99989	428.99970	0.45
C ₁₅ H ₁₁ Cl ₂ O ₁₁	436.96842	436.96840	0.06
C ₁₅ H ₁₃ Cl ₂ O ₁₁	438.98374	438.98405	-0.69
C ₁₅ H ₁₅ Cl ₂ O ₁₁	440.99969	440.99970	-0.01
C ₁₆ H ₁₁ Cl ₂ O ₁₁	448.96840	448.96840	0
C ₁₆ H ₁₃ Cl ₂ O ₁₁	450.98404	450.98405	-0.01
C ₁₆ H ₁₅ Cl ₂ O ₁₁	452.99950	452.99970	-0.43

$C_{17}H_{13}Cl_2O_{11}$	462.98407	462.98405	0.05
$C_{17}H_{15}Cl_2O_{11}$	464.99962	464.99970	-0.16
$C_{17}H_{17}Cl_2O_{11}$	467.01540	467.01535	0.12
$C_{17}H_{19}Cl_2O_{11}$	469.03135	469.03100	0.76
$C_{18}H_{15}Cl_2O_{11}$	476.99962	476.99970	-0.16
$C_{18}H_{17}Cl_2O_{11}$	479.01545	479.01535	0.22

Table S3 Chlorine containing products in Taihe sample with the same formula of previously reported DBPs

compound ^a	Formula ^{a,b}	structure ^a	theoretical mass ^{a,b}	measured mass ^b	error (ppm)
chlorohydroxybenzene dicarboxylic acid	C ₈ H ₅ ClO ₅		215.98255	215.98254	-0.06
dichlorohydroxybenzene dicarboxylic acid	C ₈ H ₄ Cl ₂ O ₅		249.94358	249.94377	0.74
chlorohydroxybenzene tricarboxylic acid	C ₉ H ₅ ClO ₇		259.97238	259.97238	0
2,2-dichlorohexanedioic acid	C ₆ H ₈ Cl ₂ O ₄		213.97996	213.97996	0
2,2-dichlorooctanedioic acid	C ₈ H ₁₂ Cl ₂ O ₄		242.01126	242.01132	0.23
dichlorooctenedioic acid	C ₈ H ₁₀ Cl ₂ O ₄		239.99561	239.99558	-0.14
2-chlorononanedioic acid	C ₉ H ₁₅ ClO ₄		222.06589	222.06595	0.25

a. DBPs have been reported in literature.

b. chlorine containing products detected in chlorinated Taihe sample.