Supporting Information

Bromination of Marine Dissolved Organic Matter following Full Scale Electrochemical Ballast Water Disinfection

*Michael Gonsior [a], Carys Mitchelmore [a], Andrew Heyes [a], Mourad Harir [b], Susan D. Richardson [c] William Tyler Petty [c], David A. Wright [a,e] and Philippe Schmitt-Kopplin [b,d]

[a] University of Maryland Center for Environmental Science, Chesapeake Biological Laboratory, Solomons, USA

[b] Helmholtz Zentrum München, Analytical BioGeoChemistry, Neuherberg, Germany

[c] University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC, USA

[d] Technische Universität München, Analytical Food Chemistry, D-85354 Freising-Weihenstephan, Germany

[e] Environmental Research Services, Baltimore, Maryland, USA

*Corresponding author. Michael Gonsior, Chesapeake Biological Laboratory, 146 Williams Street, Solomons, MD 20688, phone: +14103267245, fax: +14103267302, Email: gonsior@umces.edu

Summary

Table S1: All newly formed DBPs during electrochemical disinfection of ballast water measured by ultrahigh resolution mass spectrometry and cross validated by isotope simulations greater 1% relative abundance. Note: Possible structures are only suggestions based on the molecular formula and only given for formulas up to 8 carbon atoms and/or multiple bromine atoms. Known DBPs are highlighted in this table in bold.

Possible structure	Mass (neutral)	Rel. abundance	Formula (neutral)	O/C	H/C	DBE	DBE/C
Dibromomethane	**171.8523**	**1.4**	**C1H2Br2**	**0.00**	**2.00**	**0**	**0.00**
BromoHCD	**189.9266**	**1.7**	**C5H3O3Br1**	**0.60**	**0.60**	**4**	**0.80**
Bromo-benzenetriol	203.9422	1.1	C6H5O3Br1	0.50	0.83	4	0.67
Bromo-methyl-oxo-pentenoic acid	205.9579	2.7	C6H7O3Br1	0.50	1.17	3	0.50
bromo-heptenoic acid	205.9942	2.6	C7H11O2Br1	0.29	1.57	2	0.29
Bromophenylacetic acid	**213.9629**	**4.0**	**C8H7O2Br1**	**0.25**	**0.88**	**5**	**0.63**
Bromohydroxybenzoic acid	**215.9422**	**4.0**	**C7H5O3Br1**	**0.43**	**0.71**	**5**	**0.71**
Bromo-oxo-furanylidene acetic acid	217.9215	1.2	C6H3O4Br1	0.67	0.50	5	0.83
Bromo-methoxy-benzenediol	217.9579	1.2	C7H7O3Br1	0.43	1.00	4	0.57
Bromomethyl-oxo-dihydro-furancarboxylic acid	219.9371	1.5	C6H5O4Br1	0.67	0.83	4	0.67
Ethyl-bromo-oxo-pentenoate	219.9735	1.2	C7H9O3Br1	0.43	1.29	3	0.43
Bromoethoxy-oxo-butenoic acid	221.9528	2.7	C6H7O4Br1	0.67	1.17	3	0.50
	223.9473	1.6	C9H5O2Br1	0.22	0.56	7	0.78
Dibromopropenoic acid	**227.8422**	**1.5**	**C3H2O2Br2**	**0.67**	**0.67**	**2**	**0.67**
Bromo-formylbenzoic acid	227.9422	1.9	C8H5O3Br1	0.38	0.63	6	0.75
Dibromopropanoic acid	**229.8578**	**10.0**	**C3H4O2Br2**	**0.67**	**1.33**	**1**	**0.33**
Bromo-methoxybenzoic acid	229.9579	5.9	C8H7O3Br1	0.38	0.88	5	0.63
	229.9942	5.9	C9H11O2Br1	0.22	1.22	4	0.44
Bromo-dihydroxybenzoic acid	231.9371	3.0	C7H5O4Br1	0.57	0.71	5	0.71
Bromo-dimethoxyphenol	231.9735	1.9	C8H9O3Br1	0.38	1.13	4	0.50
	232.0099	1.2	C9H13O2Br1	0.22	1.44	3	0.33
	233.9164	1.3	C6H3O5Br1	0.83	0.50	5	0.83
Bromo-dihydroxy-cyclohexadiene-carboxylic acid	233.9528	3.9	C7H7O4Br1	0.57	1.00	4	0.57
	233.9892	1.1	C8H11O3Br1	0.38	1.38	3	0.38
Bromo-oxo-hexenedioic acid	235.932	1.6	C6H5O5Br1	0.83	0.83	4	0.67
Methyl-bromo-hydroxy-heptadienoate	235.9684	2.7	C7H9O4Br1	0.57	1.29	3	0.43

	239.9422	2.2	C9H5O3Br1	0.33	0.56	7	0.78
	241.9579	1.2	C9H7O3Br1	0.33	0.78	6	0.67
	241.9942	1.0	C10H11O2Br1	0.20	1.10	5	0.50
Dibromobutanoic acid	**243.8735**	**1.4**	**C4H6O2Br2**	**0.50**	**1.50**	**1**	**0.25**
Bromophthalicacid	243.9371	2.3	C8H5O4Br1	0.50	0.63	6	0.75
	243.9735	2.4	C9H9O3Br1	0.33	1.00	5	0.56
	244.0099	1.5	C10H13O2Br1	0.20	1.30	4	0.40
Bromo-hydroxy-methoxybenzoic acid	245.9528	2.7	C8H7O4Br1	0.50	0.88	5	0.63
	245.9892	3.0	C9H11O3Br1	0.33	1.22	4	0.44
Bromo-trihydroxybenzoic acid	247.932	2.5	C7H5O5Br1	0.71	0.71	5	0.71
Methyl-bromo-dihydroxy-cyclohexadiene-carboxylate	247.9684	2.4	C8H9O4Br1	0.50	1.13	4	0.50
Dibromophenol	**249.8629**	**3.9**	**C6H4O1Br2**	**0.17**	**0.67**	**4**	**0.67**
Bromo-dihydroxy-oxo-cyclohexene-carboxylic acid	249.9477	9.7	C7H7O5Br1	0.71	1.00	4	0.57
Bromo-butene-diyl diacetate	249.9841	2.1	C8H11O4Br1	0.50	1.38	3	0.38
Bromo-trihydroxy-cyclohexene-carboxylic acid	251.9633	2.6	C7H9O5Br1	0.71	1.29	3	0.43
	255.9371	1.0	C9H5O4Br1	0.44	0.56	7	0.78
	255.9735	1.8	C10H9O3Br1	0.30	0.90	6	0.60
	257.9528	2.0	C9H7O4Br1	0.44	0.78	6	0.67
	257.9892	3.1	C10H11O3Br1	0.30	1.10	5	0.50
	259.932	2.2	C8H5O5Br1	0.63	0.63	6	0.75
	259.9684	3.7	C9H9O4Br1	0.44	1.00	5	0.56
	260.0048	1.0	C10H13O3Br1	0.30	1.30	4	0.40
	261.9477	2.0	C8H7O5Br1	0.63	0.88	5	0.63
	261.9841	2.6	C9H11O4Br1	0.44	1.22	4	0.44
Methyl-bromo-dihydroxy-oxo-cyclohexene-carboxylate	263.9633	4.1	C8H9O5Br1	0.63	1.13	4	0.50
	263.9997	1.5	C9H13O4Br1	0.44	1.44	3	0.33
	265.9426	5.4	C7H7O6Br1	0.86	1.00	4	0.57
	265.979	2.4	C8H11O5Br1	0.63	1.38	3	0.38
Dibromo HCD	**267.8371**	**9.7**	**C5H2O3Br2**	**0.60**	**0.40**	**4**	**0.80**
	267.9371	2.0	C10H5O4Br1	0.40	0.50	8	0.80
	267.9946	1.1	C8H13O5Br1	0.63	1.63	2	0.25
Dibromo-oxopentenoic acid	269.8527	1.5	C5H4O3Br2	0.60	0.80	3	0.60
	269.9528	1.0	C10H7O4Br1	0.40	0.70	7	0.70
	269.9892	1.0	C11H11O3Br1	0.27	1.00	6	0.55
	271.9684	2.8	C10H9O4Br1	0.40	0.90	6	0.60
	272.0048	1.1	C11H13O3Br1	0.27	1.18	5	0.45
	273.9477	2.9	C9H7O5Br1	0.56	0.78	6	0.67

Tribromo-propene	275.7785	1.1	C3H3Br3	0.00	1.00	1	0.33
	275.927	1.1	C8H5O6Br1	0.75	0.63	6	0.75
	275.9633	4.0	C9H9O5Br1	0.56	1.00	5	0.56
	275.9997	2.5	C10H13O4Br1	0.40	1.30	4	0.40
	277.9426	1.6	C8H7O6Br1	0.75	0.88	5	0.63
	277.979	3.0	C9H11O5Br1	0.56	1.22	4	0.44
	278.0154	1.4	C10H15O4Br1	0.40	1.50	3	0.30
	279.9583	1.9	C8H9O6Br1	0.75	1.13	4	0.50
	279.9946	2.7	C9H13O5Br1	0.56	1.44	3	0.33
	281.9528	1.4	C11H7O4Br1	0.36	0.64	8	0.73
	281.9739	1.3	C8H11O6Br1	0.75	1.38	3	0.38
	281.9892	1.4	C12H11O3Br1	0.25	0.92	7	0.58
	283.932	4.2	C10H5O5Br1	0.50	0.50	8	0.80
	283.9684	1.4	C11H9O4Br1	0.36	0.82	7	0.64
Dibromopentenedioic acid	**285.8476**	**1.4**	**C5H4O4Br2**	**0.80**	**0.80**	**3**	**0.60**
	285.9477	1.7	C10H7O5Br1	0.50	0.70	7	0.70
	285.9841	1.6	C11H11O4Br1	0.36	1.00	6	0.55
	287.927	1.1	C9H5O6Br1	0.67	0.56	7	0.78
	287.9633	2.4	C10H9O5Br1	0.50	0.90	6	0.60
	287.9997	13.8	C11H13O4Br1	0.36	1.18	5	0.45
	289.9426	1.8	C9H7O6Br1	0.67	0.78	6	0.67
	289.979	4.3	C10H11O5Br1	0.50	1.10	5	0.50
	290.0154	1.5	C11H15O4Br1	0.36	1.36	4	0.36
	291.9583	3.0	C9H9O6Br1	0.67	1.00	5	0.56
	291.9946	4.2	C10H13O5Br1	0.50	1.30	4	0.40
	292.031	1.5	C11H17O4Br1	0.36	1.55	3	0.27
	293.9528	1.0	C12H7O4Br1	0.33	0.58	9	0.75
	293.9739	3.2	C9H11O6Br1	0.67	1.22	4	0.44
	294.0103	2.0	C10H15O5Br1	0.50	1.50	3	0.30
Dibromo-dihydroxyquinone	295.8320	1.2	C6H2O4Br2	0.67	0.33	5	0.83
	295.9320	1.3	C11H5O5Br1	0.45	0.45	9	0.82
	295.9684	1.0	C12H9O4Br1	0.33	0.75	8	0.67
	295.9896	3.6	C9H13O6Br1	0.67	1.44	3	0.33
	297.9477	1.5	C11H7O5Br1	0.45	0.64	8	0.73
	297.9841	1.3	C12H11O4Br1	0.33	0.92	7	0.58
	299.9633	2.1	C11H9O5Br1	0.45	0.82	7	0.64
	299.9997	1.5	C12H13O4Br1	0.33	1.08	6	0.50
	300.0361	1.4	C13H17O3Br1	0.23	1.31	5	0.38
	301.9426	1.7	C10H7O6Br1	0.60	0.70	7	0.70
	301.979	3.0	C11H11O5Br1	0.45	1.00	6	0.55
	302.0154	3.3	C12H15O4Br1	0.33	1.25	5	0.42
	303.9583	2.5	C10H9O6Br1	0.60	0.90	6	0.60
	303.9946	5.5	C11H13O5Br1	0.45	1.18	5	0.45
	304.031	1.5	C12H17O4Br1	0.33	1.42	4	0.33

	305.9739	4.5	C10H11O6Br1	0.60	1.10	5	0.50
	306.0103	3.9	C11H15O5Br1	0.45	1.36	4	0.36
Dibromo-methoxybenzoic acid	307.8684	2.7	C8H6O3Br2	0.38	0.75	5	0.63
	307.9532	3.1	C9H9O7Br1	0.78	1.00	5	0.56
	307.9896	5.1	C10H13O6Br1	0.60	1.30	4	0.40
	308.0259	1.5	C11H17O5Br1	0.45	1.55	3	0.27
Dibromo-dihydroxybenzoic acid	309.8476	1.3	C7H4O4Br2	0.57	0.57	5	0.71
	309.9477	1.0	C12H7O5Br1	0.42	0.58	9	0.75
	310.0052	1.7	C10H15O6Br1	0.60	1.50	3	0.30
	311.8269	4.8	C6H2O5Br2	0.83	0.33	5	0.83
	311.927	1.9	C11H5O6Br1	0.55	0.45	9	0.82
	311.9633	1.2	C12H9O5Br1	0.42	0.75	8	0.67
	313.9426	1.0	C11H7O6Br1	0.55	0.64	8	0.73
	313.979	1.7	C12H11O5Br1	0.42	0.92	7	0.58
	314.0154	1.4	C13H15O4Br1	0.31	1.15	6	0.46
	315.9583	1.8	C11H9O6Br1	0.55	0.82	7	0.64
	315.9946	2.3	C12H13O5Br1	0.42	1.08	6	0.50
	316.031	1.3	C13H17O4Br1	0.31	1.31	5	0.38
	317.9375	1.3	C10H7O7Br1	0.70	0.70	7	0.70
	317.9739	3.5	C11H11O6Br1	0.55	1.00	6	0.55
	318.0103	5.2	C12H15O5Br1	0.42	1.25	5	0.42
	318.0467	1.1	C13H19O4Br1	0.31	1.46	4	0.31
	319.9532	2.0	C10H9O7Br1	0.70	0.90	6	0.60
	319.9896	4.5	C11H13O6Br1	0.55	1.18	5	0.45
	320.0259	2.7	C12H17O5Br1	0.42	1.42	4	0.33
	321.9688	2.7	C10H11O7Br1	0.70	1.10	5	0.50
	322.0052	3.7	C11H15O6Br1	0.55	1.36	4	0.36
	322.0416	1.1	C12H19O5Br1	0.42	1.58	3	0.25
Dibromo-trimethoxybenzene	323.8997	1.3	C9H10O3Br2	0.33	1.11	4	0.44
	323.9845	1.9	C10H13O7Br1	0.70	1.30	4	0.40
	324.0209	1.9	C11H17O6Br1	0.55	1.55	3	0.27
	325.9426	1.3	C12H7O6Br1	0.50	0.58	9	0.75
	325.979	1.0	C13H11O5Br1	0.38	0.85	8	0.62
	327.9219	2.2	C11H5O7Br1	0.64	0.45	9	0.82
	327.9583	2.1	C12H9O6Br1	0.50	0.75	8	0.67
	327.9946	1.5	C13H13O5Br1	0.38	1.00	7	0.54
	329.9375	1.0	C11H7O7Br1	0.64	0.64	8	0.73
	329.9739	2.3	C12H11O6Br1	0.50	0.92	7	0.58
	330.0103	2.2	C13H15O5Br1	0.38	1.15	6	0.46
	331.9532	1.7	C11H9O7Br1	0.64	0.82	7	0.64
	331.9896	3.7	C12H13O6Br1	0.50	1.08	6	0.50
	332.0259	3.5	C13H17O5Br1	0.38	1.31	5	0.38
	333.9688	3.3	C11H11O7Br1	0.64	1.00	6	0.55
	334.0052	5.5	C12H15O6Br1	0.50	1.25	5	0.42

	334.0416	2.0	C13H19O5Br1	0.38	1.46	4	0.31
	335.9481	1.1	C10H9O8Br1	0.80	0.90	6	0.60
	335.9845	3.9	C11H13O7Br1	0.64	1.18	5	0.45
	336.0209	3.5	C12H17O6Br1	0.50	1.42	4	0.33
Dibromo-dimethoxybenzoic acid	337.8789	1.0	C9H8O4Br2	0.44	0.89	5	0.56
	337.9637	1.0	C10H11O8Br1	0.80	1.10	5	0.50
	338.0001	2.6	C11H15O7Br1	0.64	1.36	4	0.36
	338.0365	1.9	C12H19O6Br1	0.50	1.58	3	0.25
	339.9583	1.5	C13H9O6Br1	0.46	0.69	9	0.69
	339.9946	1.4	C14H13O5Br1	0.36	0.93	8	0.57
	340.0158	1.2	C11H17O7Br1	0.64	1.55	3	0.27
Tribromo-ethene-sulfonate	341.7196	4.1	C2H1Br3O3S	1.50	0.50	1	0.50
	341.9375	1.1	C12H7O7Br1	0.58	0.58	9	0.75
	341.9739	2.1	C13H11O6Br1	0.46	0.85	8	0.62
	342.0103	1.4	C14H15O5Br1	0.36	1.07	7	0.50
	343.9532	1.9	C12H9O7Br1	0.58	0.75	8	0.67
	343.9896	3.0	C13H13O6Br1	0.46	1.00	7	0.54
	344.0259	2.4	C14H17O5Br1	0.36	1.21	6	0.43
TribromoHCD	**345.7476**	**21.5**	**C5H1O3Br3**	**0.60**	**0.20**	**4**	**0.80**
	345.9688	2.5	C12H11O7Br1	0.58	0.92	7	0.58
	346.0052	4.4	C13H15O6Br1	0.46	1.15	6	0.46
	346.0416	2.9	C14H19O5Br1	0.36	1.36	5	0.36
	347.9481	1.1	C11H9O8Br1	0.73	0.82	7	0.64
	347.9845	4.4	C12H13O7Br1	0.58	1.08	6	0.50
	348.0209	5.3	C13H17O6Br1	0.46	1.31	5	0.38
	348.0572	2.2	C14H21O5Br1	0.36	1.50	4	0.29
	349.9637	2.2	C11H11O8Br1	0.73	1.00	6	0.55
	350.0001	5.1	C12H15O7Br1	0.58	1.25	5	0.42
	350.0365	3.4	C13H19O6Br1	0.46	1.46	4	0.31
	351.9794	2.2	C11H13O8Br1	0.73	1.18	5	0.45
	352.0158	3.8	C12H17O7Br1	0.58	1.42	4	0.33
	352.0522	1.7	C13H21O6Br1	0.46	1.62	3	0.23
	353.9375	1.1	C13H7O7Br1	0.54	0.54	10	0.77
	353.9739	1.3	C14H11O6Br1	0.43	0.79	9	0.64
	353.995	1.2	C11H15O8Br1	0.73	1.36	4	0.36
	354.0103	1.4	C15H15O5Br1	0.33	1.00	8	0.53
	354.0314	2.1	C12H19O7Br1	0.58	1.58	3	0.25
	355.9168	1.1	C12H5O8Br1	0.67	0.42	10	0.83
	355.9532	1.5	C13H9O7Br1	0.54	0.69	9	0.69
	355.9896	2.3	C14H13O6Br1	0.43	0.93	8	0.57
	356.0259	1.4	C15H17O5Br1	0.33	1.13	7	0.47
	357.9688	2.3	C13H11O7Br1	0.54	0.85	8	0.62
	358.0052	3.0	C14H15O6Br1	0.43	1.07	7	0.50
	358.0416	3.1	C15H19O5Br1	0.33	1.27	6	0.40
	359.9481	1.0	C12H9O8Br1	0.67	0.75	8	0.67

	359.9845	3.6	C13H13O7Br1	0.54	1.00	7	0.54
	360.0209	4.5	C14H17O6Br1	0.43	1.21	6	0.43
	360.0572	2.7	C15H21O5Br1	0.33	1.40	5	0.33
	361.9637	2.0	C12H11O8Br1	0.67	0.92	7	0.58
	362.0001	5.1	C13H15O7Br1	0.54	1.15	6	0.46
	362.0365	4.9	C14H19O6Br1	0.43	1.36	5	0.36
	362.0729	1.5	C15H23O5Br1	0.33	1.53	4	0.27
	363.9794	3.4	C12H13O8Br1	0.67	1.08	6	0.50
	364.0158	5.7	C13H17O7Br1	0.54	1.31	5	0.38
	364.0522	3.1	C14H21O6Br1	0.43	1.50	4	0.29
	365.995	3.2	C12H15O8Br1	0.67	1.25	5	0.42
	366.0314	3.5	C13H19O7Br1	0.54	1.46	4	0.31
	366.0678	1.4	C14H23O6Br1	0.43	1.64	3	0.21
	367.8531	1.0	C9H6O6Br2	0.67	0.67	6	0.67
	367.9532	1.0	C14H9O7Br1	0.50	0.64	10	0.71
	367.9896	1.1	C15H13O6Br1	0.40	0.87	9	0.60
	368.0107	1.8	C12H17O8Br1	0.67	1.42	4	0.33
	368.0471	1.8	C13H21O7Br1	0.54	1.62	3	0.23
	369.9688	1.7	C14H11O7Br1	0.50	0.79	9	0.64
	370.0052	2.4	C15H15O6Br1	0.40	1.00	8	0.53
	370.0416	1.4	C16H19O5Br1	0.31	1.19	7	0.44
	371.8844	1.2	C9H10O6Br2	0.67	1.11	4	0.44
	371.9481	1.3	C13H9O8Br1	0.62	0.69	9	0.69
	371.9845	2.7	C14H13O7Br1	0.50	0.93	8	0.57
	372.0209	3.2	C15H17O6Br1	0.40	1.13	7	0.47
	372.0572	1.9	C16H21O5Br1	0.31	1.31	6	0.38
Tribromo-methoxy-benzenediol	373.7789	1.1	C7H5O3Br3	0.43	0.71	4	0.57
	373.9637	1.7	C13H11O8Br1	0.62	0.85	8	0.62
	374.0001	4.3	C14H15O7Br1	0.50	1.07	7	0.50
	374.0365	4.6	C15H19O6Br1	0.40	1.27	6	0.40
	374.0729	1.4	C16H23O5Br1	0.31	1.44	5	0.31
	375.9794	3.3	C13H13O8Br1	0.62	1.00	7	0.54
	376.0158	6.2	C14H17O7Br1	0.50	1.21	6	0.43
	377.9586	1.3	C12H11O9Br1	0.75	0.92	7	0.58
	377.995	5.0	C13H15O8Br1	0.62	1.15	6	0.46
	378.0314	5.5	C14H19O7Br1	0.50	1.36	5	0.36
	378.0678	2.8	C15H23O6Br1	0.40	1.53	4	0.27
	379.9743	1.6	C12H13O9Br1	0.75	1.08	6	0.50
	380.0107	3.9	C13H17O8Br1	0.62	1.31	5	0.38
	380.0471	3.4	C14H21O7Br1	0.50	1.50	4	0.29
	381.9899	1.0	C12H15O9Br1	0.75	1.25	5	0.42
	382.0263	2.4	C13H19O8Br1	0.62	1.46	4	0.31
	382.0627	1.7	C14H23O7Br1	0.50	1.64	3	0.21
	383.8844	1.1	C10H10O6Br2	0.60	1.00	5	0.50
	383.9481	1.1	C14H9O8Br1	0.57	0.64	10	0.71

	383.9845	1.6	C15H13O7Br1	0.47	0.87	9	0.60
	384.0209	2.0	C16H17O6Br1	0.38	1.06	8	0.50
	384.0572	1.1	C17H21O5Br1	0.29	1.24	7	0.41
	385.9637	1.9	C14H11O8Br1	0.57	0.79	9	0.64
	386.0001	4.8	C15H15O7Br1	0.47	1.00	8	0.53
	386.0365	3.3	C16H19O6Br1	0.38	1.19	7	0.44
	386.0729	1.6	C17H23O5Br1	0.29	1.35	6	0.35
	387.9794	2.8	C14H13O8Br1	0.57	0.93	8	0.57
	388.0158	5.2	C15H17O7Br1	0.47	1.13	7	0.47
	388.0522	4.2	C16H21O6Br1	0.38	1.31	6	0.38
	388.0885	2.0	C17H25O5Br1	0.29	1.47	5	0.29
	389.9586	1.2	C13H11O9Br1	0.69	0.85	8	0.62
	389.995	4.9	C14H15O8Br1	0.57	1.07	7	0.50
	390.0314	6.6	C15H19O7Br1	0.47	1.27	6	0.40
	390.1042	6.7	C17H27O5Br1	0.29	1.59	4	0.24
	391.9743	2.3	C13H13O9Br1	0.69	1.00	7	0.54
	392.0107	5.9	C14H17O8Br1	0.57	1.21	6	0.43
	392.0835	2.1	C16H25O6Br1	0.38	1.56	4	0.25
	393.9899	2.7	C13H15O9Br1	0.69	1.15	6	0.46
	394.0263	4.9	C14H19O8Br1	0.57	1.36	5	0.36
	394.0627	3.3	C15H23O7Br1	0.47	1.53	4	0.27
	396.0056	1.6	C13H17O9Br1	0.69	1.31	5	0.38
	396.042	2.3	C14H21O8Br1	0.57	1.50	4	0.29
	397.9001	1.3	C11H12O6Br2	0.55	1.09	5	0.45
	397.9637	1.1	C15H11O8Br1	0.53	0.73	10	0.67
	398.0001	1.3	C16H15O7Br1	0.44	0.94	9	0.56
	398.0365	1.5	C17H19O6Br1	0.35	1.12	8	0.47
	399.8793	1.1	C10H10O7Br2	0.70	1.00	5	0.50
	399.9794	2.1	C15H13O8Br1	0.53	0.87	9	0.60
	400.0158	3.2	C16H17O7Br1	0.44	1.06	8	0.50
	400.0522	3.0	C17H21O6Br1	0.35	1.24	7	0.41
	400.0885	1.2	C18H25O5Br1	0.28	1.39	6	0.33
	401.9586	1.5	C14H11O9Br1	0.64	0.79	9	0.64
	401.995	4.0	C15H15O8Br1	0.53	1.00	8	0.53
	402.0314	5.3	C16H19O7Br1	0.44	1.19	7	0.44
	402.0678	3.7	C17H23O6Br1	0.35	1.35	6	0.35
	403.9743	2.6	C14H13O9Br1	0.64	0.93	8	0.57
	404.0107	7.6	C15H17O8Br1	0.53	1.13	7	0.47
	404.0835	4.2	C17H25O6Br1	0.35	1.47	5	0.29
	405.9899	3.8	C14H15O9Br1	0.64	1.07	7	0.50
	406.0263	7.0	C15H19O8Br1	0.53	1.27	6	0.40
	406.0991	3.9	C17H27O6Br1	0.35	1.59	4	0.24
	408.0056	3.9	C14H17O9Br1	0.64	1.21	6	0.43
	408.042	5.0	C15H21O8Br1	0.53	1.40	5	0.33
	408.0784	2.9	C16H25O7Br1	0.44	1.56	4	0.25
	410.0212	2.4	C14H19O9Br1	0.64	1.36	5	0.36

	410.0576	2.9	C15H23O8Br1	0.53	1.53	4	0.27
	411.9157	1.0	C12H14O6Br2	0.50	1.17	5	0.42
	411.9794	1.0	C16H13O8Br1	0.50	0.81	10	0.63
	412.0158	1.5	C17H17O7Br1	0.41	1.00	9	0.53
	412.0369	1.1	C14H21O9Br1	0.64	1.50	4	0.29
	412.0522	1.7	C18H21O6Br1	0.33	1.17	8	0.44
	412.0733	1.1	C15H25O8Br1	0.53	1.67	3	0.20
	413.9586	1.1	C15H11O9Br1	0.60	0.73	10	0.67
	413.995	2.1	C16H15O8Br1	0.50	0.94	9	0.56
	414.0314	3.1	C17H19O7Br1	0.41	1.12	8	0.47
	414.0678	2.6	C18H23O6Br1	0.33	1.28	7	0.39
	415.9743	1.9	C15H13O9Br1	0.60	0.87	9	0.60
	416.0107	4.2	C16H17O8Br1	0.50	1.06	8	0.50
	416.0471	5.0	C17H21O7Br1	0.41	1.24	7	0.41
	416.0835	3.0	C18H25O6Br1	0.33	1.39	6	0.33
	417.9899	3.6	C15H15O9Br1	0.60	1.00	8	0.53
	418.0263	9.3	C16H19O8Br1	0.50	1.19	7	0.44
	418.0991	2.3	C18H27O6Br1	0.33	1.50	5	0.28
	419.9692	1.6	C14H13O10Br1	0.71	0.93	8	0.57
	420.0056	5.3	C15H17O9Br1	0.60	1.13	7	0.47
	420.0784	4.7	C17H25O7Br1	0.41	1.47	5	0.29
	421.9849	2.2	C14H15O10Br1	0.71	1.07	7	0.50
	422.0212	4.9	C15H19O9Br1	0.60	1.27	6	0.40
	424.0369	3.2	C15H21O9Br1	0.60	1.40	5	0.33
	424.0733	2.6	C16H25O8Br1	0.50	1.56	4	0.25
	425.995	1.2	C17H15O8Br1	0.47	0.88	10	0.59
	426.0314	1.7	C18H19O7Br1	0.39	1.06	9	0.50
	426.0678	1.7	C19H23O6Br1	0.32	1.21	8	0.42
	427.9743	1.4	C16H13O9Br1	0.56	0.81	10	0.63
	428.0107	3.1	C17H17O8Br1	0.47	1.00	9	0.53
	428.0471	3.4	C18H21O7Br1	0.39	1.17	8	0.44
	428.0835	2.4	C19H25O6Br1	0.32	1.32	7	0.37
	429.9899	2.7	C16H15O9Br1	0.56	0.94	9	0.56
	430.0263	4.9	C17H19O8Br1	0.47	1.12	8	0.47
	430.0991	2.7	C19H27O6Br1	0.32	1.42	6	0.32
	431.9692	1.8	C15H13O10Br1	0.67	0.87	9	0.60
	432.0056	4.9	C16H17O9Br1	0.56	1.06	8	0.50
	432.1148	1.9	C19H29O6Br1	0.32	1.53	5	0.26
	433.9849	2.9	C15H15O10Br1	0.67	1.00	8	0.53
	434.0212	6.7	C16H19O9Br1	0.56	1.19	7	0.44
	434.094	4.1	C18H27O7Br1	0.39	1.50	5	0.28
	436.0005	3.4	C15H17O10Br1	0.67	1.13	7	0.47
	436.0369	6.0	C16H21O9Br1	0.56	1.31	6	0.38
	436.0733	4.8	C17H25O8Br1	0.47	1.47	5	0.29
	438.0525	3.8	C16H23O9Br1	0.56	1.44	5	0.31
	438.0889	2.4	C17H27O8Br1	0.47	1.59	4	0.24

	440.0107	1.6	C18H17O8Br1	0.44	0.94	10	0.56
	440.0471	1.9	C19H21O7Br1	0.37	1.11	9	0.47
	440.0682	1.7	C16H25O9Br1	0.56	1.56	4	0.25
	441.9899	1.7	C17H15O9Br1	0.53	0.88	10	0.59
	442.0263	3.2	C18H19O8Br1	0.44	1.06	9	0.50
	442.0627	3.9	C19H23O7Br1	0.37	1.21	8	0.42
	443.9692	1.5	C16H13O10Br1	0.63	0.81	10	0.63
	444.0056	3.8	C17H17O9Br1	0.53	1.00	9	0.53
	444.042	6.6	C18H21O8Br1	0.44	1.17	8	0.44
	444.1148	2.1	C20H29O6Br1	0.30	1.45	6	0.30
	445.9849	2.7	C16H15O10Br1	0.63	0.94	9	0.56
	446.0212	6.4	C17H19O9Br1	0.53	1.12	8	0.47
	446.094	4.9	C19H27O7Br1	0.37	1.42	6	0.32
	448.0005	4.3	C16H17O10Br1	0.63	1.06	8	0.50
	448.0369	7.3	C17H21O9Br1	0.53	1.24	7	0.41
	450.0162	4.4	C16H19O10Br1	0.63	1.19	7	0.44
	450.0525	6.1	C17H23O9Br1	0.53	1.35	6	0.35
	450.0889	4.2	C18H27O8Br1	0.44	1.50	5	0.28
	452.0318	3.3	C16H21O10Br1	0.63	1.31	6	0.38
	452.0682	3.4	C17H25O9Br1	0.53	1.47	5	0.29
	454.0627	1.8	C20H23O7Br1	0.35	1.15	9	0.45
	456.0056	1.7	C18H17O9Br1	0.50	0.94	10	0.56
	456.042	3.2	C19H21O8Br1	0.42	1.11	9	0.47
	456.0784	3.1	C20H25O7Br1	0.35	1.25	8	0.40
	457.9849	1.6	C17H15O10Br1	0.59	0.88	10	0.59
	458.0212	3.8	C18H19O9Br1	0.50	1.06	9	0.50
	458.1304	1.5	C21H31O6Br1	0.29	1.48	6	0.29
	460.0005	3.4	C17H17O10Br1	0.59	1.00	9	0.53
	460.0369	6.7	C18H21O9Br1	0.50	1.17	8	0.44
	460.1097	3.7	C20H29O7Br1	0.35	1.45	6	0.30
	461.9798	1.7	C16H15O11Br1	0.69	0.94	9	0.56
	462.0162	5.2	C17H19O10Br1	0.59	1.12	8	0.47
	463.9954	2.3	C16H17O11Br1	0.69	1.06	8	0.50
	464.0318	5.2	C17H21O10Br1	0.59	1.24	7	0.41
	466.0475	3.5	C17H23O10Br1	0.59	1.35	6	0.35
	466.0838	3.2	C18H27O9Br1	0.50	1.50	5	0.28
	469.9212	1.0	C14H16O8Br2	0.57	1.14	6	0.43
	470.0212	1.9	C19H19O9Br1	0.47	1.00	10	0.53
	470.0576	3.0	C20H23O8Br1	0.40	1.15	9	0.45
	470.094	2.2	C21H27O7Br1	0.33	1.29	8	0.38
	472.0005	2.1	C18H17O10Br1	0.56	0.94	10	0.56
	472.0369	3.8	C19H21O9Br1	0.47	1.11	9	0.47
	472.1097	2.3	C21H29O7Br1	0.33	1.38	7	0.33
	473.9798	1.4	C17H15O11Br1	0.65	0.88	10	0.59
	474.0162	3.8	C18H19O10Br1	0.56	1.06	9	0.50
	474.0525	6.1	C19H23O9Br1	0.47	1.21	8	0.42

	474.1253	1.7	C21H31O7Br1	0.33	1.48	6	0.29
	475.9954	2.4	C17H17O11Br1	0.65	1.00	9	0.53
	476.0318	5.2	C18H21O10Br1	0.56	1.17	8	0.44
	476.1046	4.0	C20H29O8Br1	0.40	1.45	6	0.30
	478.0111	2.7	C17H19O11Br1	0.65	1.12	8	0.47
	478.0475	4.7	C18H23O10Br1	0.56	1.28	7	0.39
	480.0995	2.3	C19H29O9Br1	0.47	1.53	5	0.26
	484.0369	1.8	C20H21O9Br1	0.45	1.05	10	0.50
	484.0733	2.0	C21H25O8Br1	0.38	1.19	9	0.43
	485.9798	1.1	C18H15O11Br1	0.61	0.83	11	0.61
	486.0162	2.0	C19H19O10Br1	0.53	1.00	10	0.53
	486.0525	3.6	C20H23O9Br1	0.45	1.15	9	0.45
	486.1253	1.4	C22H31O7Br1	0.32	1.41	7	0.32
	487.9954	1.9	C18H17O11Br1	0.61	0.94	10	0.56
	488.0318	3.7	C19H21O10Br1	0.53	1.11	9	0.47
	488.0682	5.3	C20H25O9Br1	0.45	1.25	8	0.40
	490.0111	2.5	C18H19O11Br1	0.61	1.06	9	0.50
	490.0475	4.9	C19H23O10Br1	0.53	1.21	8	0.42
	490.1202	2.2	C21H31O8Br1	0.38	1.48	6	0.29
	491.9903	1.1	C17H17O12Br1	0.71	1.00	9	0.53
	492.0267	3.0	C18H21O11Br1	0.61	1.17	8	0.44
	492.0631	4.4	C19H25O10Br1	0.53	1.32	7	0.37
	492.0995	3.4	C20H29O9Br1	0.45	1.45	6	0.30
	494.0424	2.3	C18H23O11Br1	0.61	1.28	7	0.39
	494.0788	2.6	C19H27O10Br1	0.53	1.42	6	0.32
	496.0944	1.0	C19H29O10Br1	0.53	1.53	5	0.26
	498.0889	1.6	C22H27O8Br1	0.36	1.23	9	0.41
	500.0318	1.6	C20H21O10Br1	0.50	1.05	10	0.50
	500.0682	2.6	C21H25O9Br1	0.43	1.19	9	0.43
	500.1046	2.0	C22H29O8Br1	0.36	1.32	8	0.36
	502.0111	1.6	C19H19O11Br1	0.58	1.00	10	0.53
	502.0475	3.2	C20H23O10Br1	0.50	1.15	9	0.45
	502.0838	3.3	C21H27O9Br1	0.43	1.29	8	0.38
	502.1202	1.6	C22H31O8Br1	0.36	1.41	7	0.32
	504.0267	2.4	C19H21O11Br1	0.58	1.11	9	0.47
	504.0631	3.7	C20H25O10Br1	0.50	1.25	8	0.40
	504.0995	3.1	C21H29O9Br1	0.43	1.38	7	0.33
	506.006	1.3	C18H19O12Br1	0.67	1.06	9	0.50
	506.0424	2.7	C19H23O11Br1	0.58	1.21	8	0.42
	506.0788	3.2	C20H27O10Br1	0.50	1.35	7	0.35
	506.1151	1.7	C21H31O9Br1	0.43	1.48	6	0.29
	508.0216	1.3	C18H21O12Br1	0.67	1.17	8	0.44
	508.058	2.0	C19H25O11Br1	0.58	1.32	7	0.37
	508.0944	2.0	C20H29O10Br1	0.50	1.45	6	0.30
	514.0475	1.8	C21H23O10Br1	0.48	1.10	10	0.48
	514.0838	2.2	C22H27O9Br1	0.41	1.23	9	0.41

	514.1202	1.4	C23H31O8Br1	0.35	1.35	8	0.35
	516.0267	1.6	C20H21O11Br1	0.55	1.05	10	0.50
	516.0631	3.0	C21H25O10Br1	0.48	1.19	9	0.43
	516.0995	2.5	C22H29O9Br1	0.41	1.32	8	0.36
	516.1359	1.2	C23H33O8Br1	0.35	1.43	7	0.30
	518.006	1.1	C19H19O12Br1	0.63	1.00	10	0.53
	518.0424	2.3	C20H23O11Br1	0.55	1.15	9	0.45
	518.0788	3.0	C21H27O10Br1	0.48	1.29	8	0.38
	518.1151	1.8	C22H31O9Br1	0.41	1.41	7	0.32
	520.0216	1.5	C19H21O12Br1	0.63	1.11	9	0.47
	520.058	2.3	C20H25O11Br1	0.55	1.25	8	0.40
	520.0944	2.3	C21H29O10Br1	0.48	1.38	7	0.33
	520.1308	1.1	C22H33O9Br1	0.41	1.50	6	0.27
	522.0373	1.2	C19H23O12Br1	0.63	1.21	8	0.42
	522.0737	1.8	C20H27O11Br1	0.55	1.35	7	0.35
	522.1101	1.1	C21H31O10Br1	0.48	1.48	6	0.29
	528.0631	1.5	C22H25O10Br1	0.45	1.14	10	0.45
	528.0995	1.4	C23H29O9Br1	0.39	1.26	9	0.39
	530.0424	1.4	C21H23O11Br1	0.52	1.10	10	0.48
	530.0788	1.9	C22H27O10Br1	0.45	1.23	9	0.41
	530.1151	1.4	C23H31O9Br1	0.39	1.35	8	0.35
	532.0216	1.1	C20H21O12Br1	0.60	1.05	10	0.50
	532.058	1.9	C21H25O11Br1	0.52	1.19	9	0.43
	532.0944	2.1	C22H29O10Br1	0.45	1.32	8	0.36
	534.0373	1.5	C20H23O12Br1	0.60	1.15	9	0.45
	534.0737	1.9	C21H27O11Br1	0.52	1.29	8	0.38
	534.1101	1.6	C22H31O10Br1	0.45	1.41	7	0.32
	536.0529	1.2	C20H25O12Br1	0.60	1.25	8	0.40
	536.0893	1.4	C21H29O11Br1	0.52	1.38	7	0.33
	544.058	1.3	C22H25O11Br1	0.50	1.14	10	0.45
	544.0944	1.3	C23H29O10Br1	0.43	1.26	9	0.39
	546.0737	1.4	C22H27O11Br1	0.50	1.23	9	0.41
	546.1101	1.2	C23H31O10Br1	0.43	1.35	8	0.35
	548.0893	1.4	C22H29O11Br1	0.50	1.32	8	0.36
	550.0686	1.1	C21H27O12Br1	0.57	1.29	8	0.38
	560.0893	1.2	C23H29O11Br1	0.48	1.26	9	0.39
	562.105	1.0	C23H31O11Br1	0.48	1.35	8	0.35