

Supporting Information:

**Multivariate Statistical Approaches for the Characterization of Dissolved Organic Matter
Analyzed by Ultrahigh Resolution Mass Spectrometry**

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Experimental, 4 Figures, 4 Tables, 25 pages total

1. Experimental

1.1. Samples and Preparation

Atlantic white cedar (*Chamaecyparis thyoides*), which has been biodegraded by brown-rot fungi, was collected from the Dismal Swamp. Because brown-rot fungi attack cellulosic components, this sample is enriched in lignin, as shown by its cross polarization magic angle spinning solid state ^{13}C nuclear magnetic resonance spectrum (1). Approximately 20 g of the ground (by mortar and pestle) biodegraded wood was extracted with 1 L of ultrapure water, shaken for 24 hr, and then 0.1 micron filtered.

The water from the transect samples was filtered through a 0.1 micron Whatman Polycap cartridge filter, while the cruise samples were filtered through double-stacked 0.7 micron precombusted glass fiber filters. DOC concentrations were determined afterwards on an Aurora 1030W total organic carbon (TOC) analyzer (wet oxidation) or a Shimadzu TOC-V_{CPH} analyzer (high temperature combustion). Dissolved inorganic carbon (DIC) was removed prior to DOC analysis by acidifying samples to a pH of 2.

For the C₁₈ extraction, disks were activated using LC-MS grade methanol (Fisher Scientific), and each water sample was acidified with HCl to a pH of 2 before passing through the disk. The amount of sample passed through each C₁₈ disk depended on the ambient concentration of DOC. Approximately 0.2 L of DS water and the WE, 0.5 L of GB and TP water, 1 L of CBB water and OSC water, and 2-6 L of water collected from Sta. 0-15 was extracted. The adsorbed DOC was rinsed with LC-MS grade water to remove residual salts before eluting off the disk with 10-20 mL of LC-MS grade methanol. Because C₁₈ extractions are routine for desalting, the extraction efficiencies of these samples were not measured. It is expected that for fresh water samples, approximately 50-60% of the DOC is recovered, while 30-

40% of the DOC is recovered for estuarine samples (salinity less than 25) and 20-30% of the DOC is recovered for marine samples (salinity greater than 25) (2-3).

The electrodialysis (ED) desalting technique uses a small volume (1.5 mL of sample) ED unit (ElectroPrep Dialysis Tank, Harvard Apparatus, Holliston, MA), where salts are removed from the sample during their movement through an electric field (200 V) through membranes (cellulose acetate, 500 Da MWCO) that separate the sample from an ultrapure water bath. Water samples were desalted by this method at their ambient concentration and pH (except for the DS water, which was diluted by 4). For samples with low DOC concentrations, the ED procedure was performed multiple times. About 1.5 mL of DS water, 3 mL of GB and TP water, 4.5 mL of CBB water, and 7.5 mL of OSC water were initially desalted with ED. Afterwards, the samples were concentrated by a rotary evaporator to 1.5 mL, and a final desalting was performed with the ED unit.

Prior to mass spectral analysis, all C₁₈ extracted samples in methanol were diluted by 2 with LC-MS grade water, while the DS-whole water (DS-WW) and WE-whole water (WE-WW), each without C₁₈ extraction, were diluted by 2 with LC-MS grade methanol, to give a final sample composition of 1:1 (v/v) water: methanol. The 5 samples prepared by ED were diluted by 25% with LC-MS grade methanol, giving a final sample composition of 3:1 (v/v) water: methanol. To increase the ionization efficiency, ammonium hydroxide was added immediately prior to electrospray (ESI), bringing the pH to 8.

1.2. Instrumentation

Samples were introduced into the ESI source by a syringe pump at an infusion rate of 120 µL/hr. The DS-WW, WE-WW, and C₁₈ extracted samples all have the highest DOC

concentrations, so ions were accumulated in a hexapole for 1.0 sec before being transferred to the ICR cell. Exactly 200 transients, collected with a 4 MWord time domain, were added. The samples prepared by ED have lower DOC concentrations, so a longer ion accumulation time of 3.0 sec was used and 300 transients were added. For all analyses, the summed free induction decay signal was zero-filled once and sine-bell apodized prior to fast Fourier transformation and magnitude calculation using the Bruker Daltonics Data Analysis software.

Approximately 84%-99% of all m/z values in each spectrum were assigned a unique molecular formula (Table S2). The total number of formulas assigned to each spectrum ranged from 1200-3000 (excluding formulas of the ^{13}C isotopes), generally with the low end associating with marine samples and the high end referring to terrestrial samples (Table S2). Average resolving powers of the broadband mass spectra are greater than 400,000, with individual peaks at the center of the m/z range at 401 having resolving powers generally exceeding 600,000.

1.3. Statistical Analysis

Hierarchical cluster analysis HCA begins by seeking out the first two samples that have the largest mutual correlations in a data matrix, and the correlations of these two samples with the rest of samples are averaged to form a new correlation matrix, from which another two samples will be sought out with the largest correlation coefficient. This procedure is repeated until a single correlation coefficient remains in the matrix. Principal component analysis (PCA), which assumes a linear relationship, can sort out a pattern of variables among the samples, whereas non-metric multi-dimensional scaling (NMS) focuses on the similarity among samples but loses relational information about the variables (4). One of the main advantages of PCA and the PCA

biplot is that the variables that are responsible for the grouping of the samples can be established, unlike NMS ordination plots that do not provide information on the variables (4).

From the molecular formula assignments, the magnitude-averaged calculations for each sample can be determined by the following equations:

$$(O/C)_w = \Sigma(O/C_n * M_n)$$

$$(H/C)_w = \Sigma(H/C_n * M_n)$$

$$DBE = 1/2 * (2\#C + \#N + \#P - \#H + 2)$$

$$(DBE)_w = \Sigma(DBE_n * M_n)$$

$$(DBE/C)_w = \Sigma(DBE/C_n * M_n)$$

$$(DBE/O)_w = \Sigma(DBE/O_n * M_n)$$

$$(C\#)_w = \Sigma(\#C_n * M_n)$$

where 'w' signifies a magnitude-weighted calculation, 'n' signifies that the parameter is calculated for each assigned formula, # represents the number of the specified atoms in the formula, and 'M' is the relative magnitude of each peak.

References

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2. Louchouart, P.; Opsahl, S.; Benner, R. Isolation and quantification of dissolved lignin from natural waters using solid-phase extraction and GC/MS. *Anal. Chem.* **2000**, *72* (13), 2780-2787.
3. Kim, S.; Simpson, A. J.; Kujawinski, E. B.; Freitas, M. A.; Hatcher, P. G. High resolution electrospray ionization mass spectrometry and 2D solution NMR for the analysis of DOM extracted by C18 solid phase disk. *Org. Geochem.*, **2003**, *34* (9), 1325-1335.
4. Lattin, J. M.; Carroll, J. D.; Green, P. E. *Analyzing multivariate data*; Thomson Brooks/Cole: Pacific Grove, 2003.

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Figure S2: van Krevelen diagrams of the 5 Chesapeake Bay transect samples desalted by electrodialysis, a) Dismal Swamp, b) Great Bridge, c) Town Point, d) Chesapeake Bay Bridge, and e) Offshore Coastal. The blue circle indicates compounds in the tannin region of the diagram (high O/C, low H/C), while the green circle indicates compounds in the carbohydrate region of the diagram (high O/C, high H/C).

Figure S3: Dendrogram from the cluster analysis using the presence/absence of the selected 2143 formulas in the 500 most abundant peaks in each sample.

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Table S4: Molecular formulas in the areas of the van Krevelen diagram shown in Figure 4. All formulas are of singly charged negative ions.

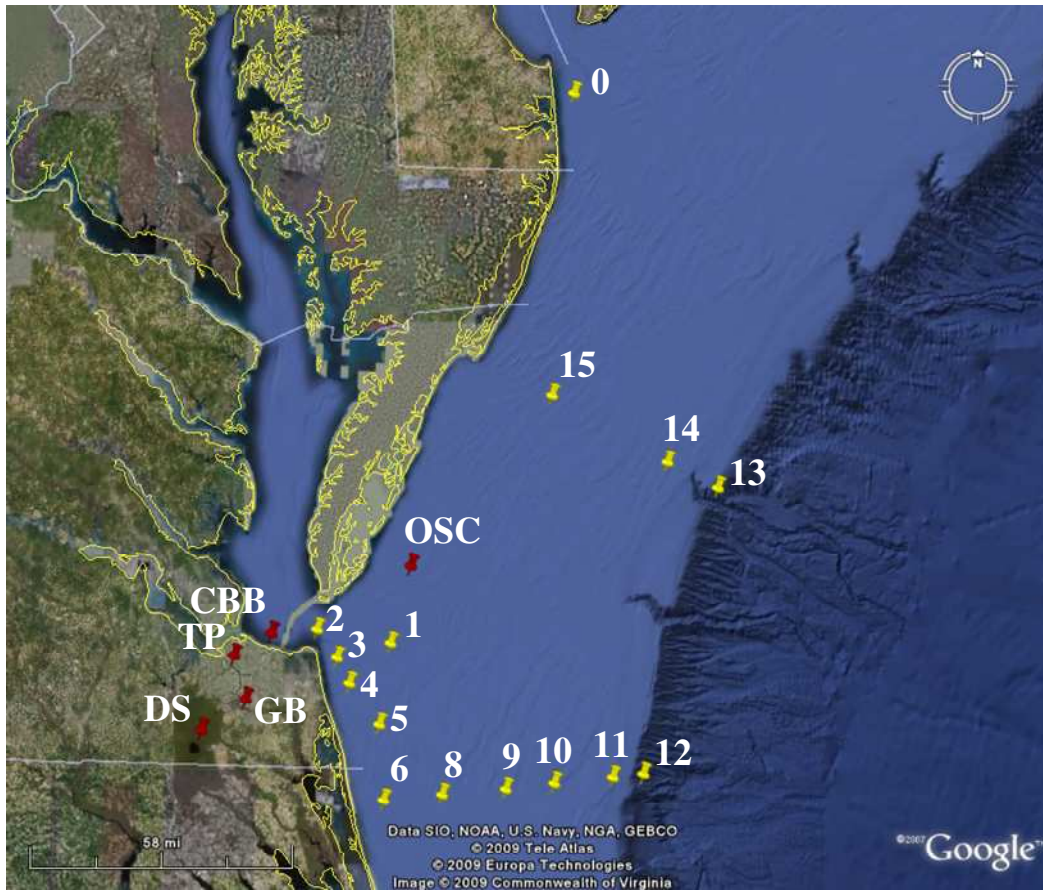


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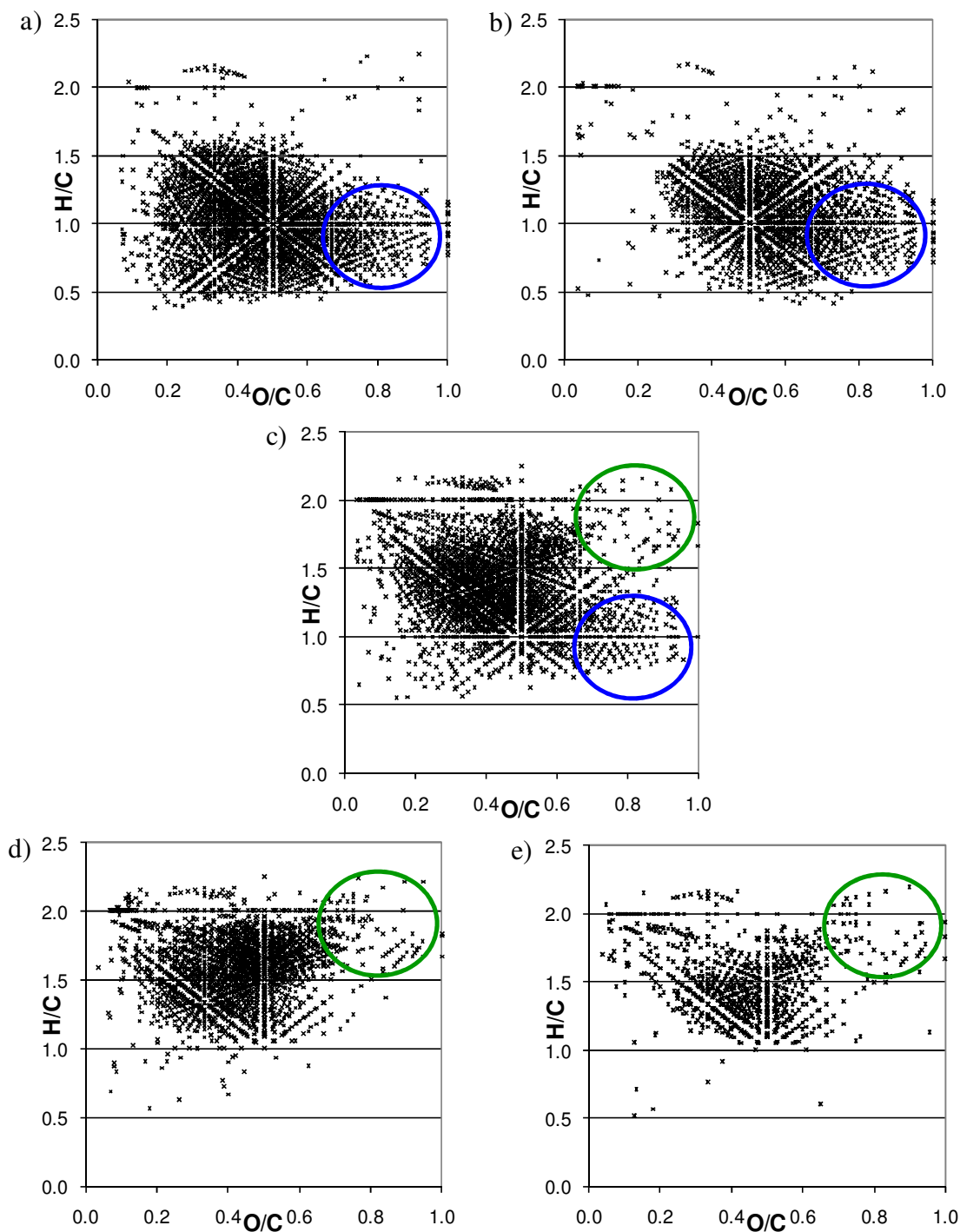


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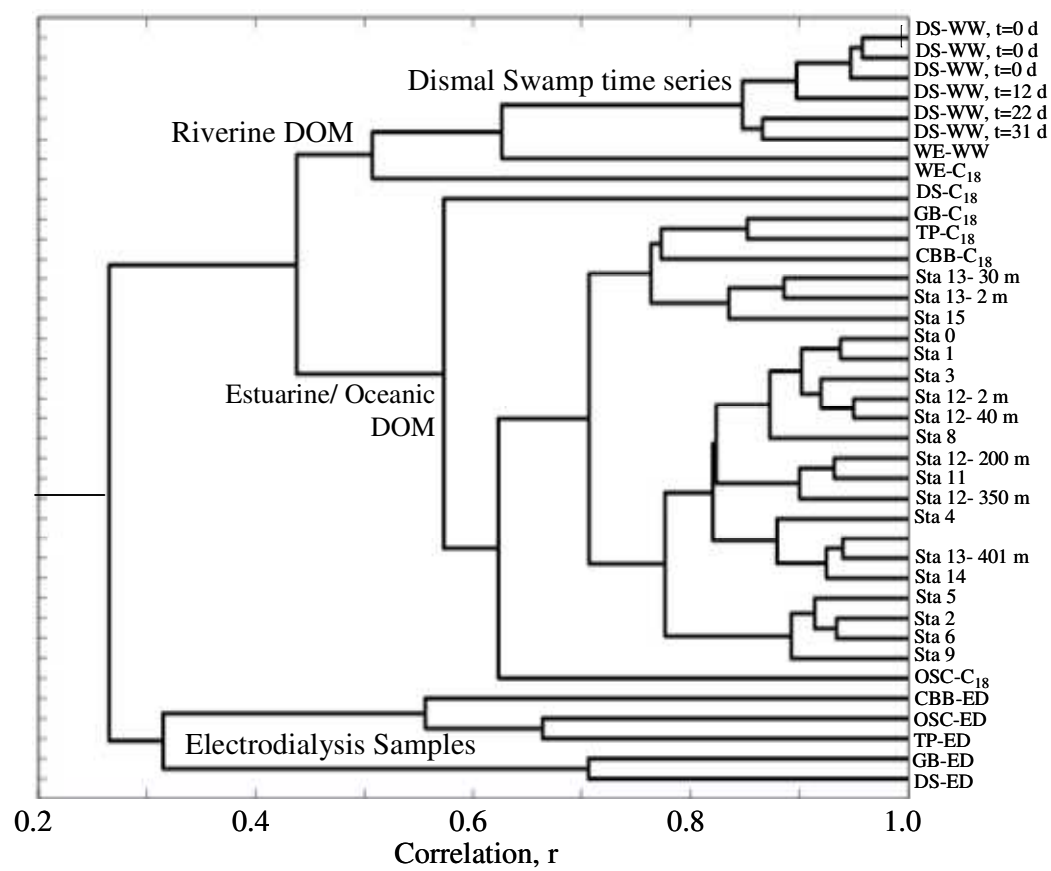


Figure S3: Dendrogram from the cluster analysis using the presence/absence of the selected 2143 formulas in the 500 most abundant peaks in each sample.

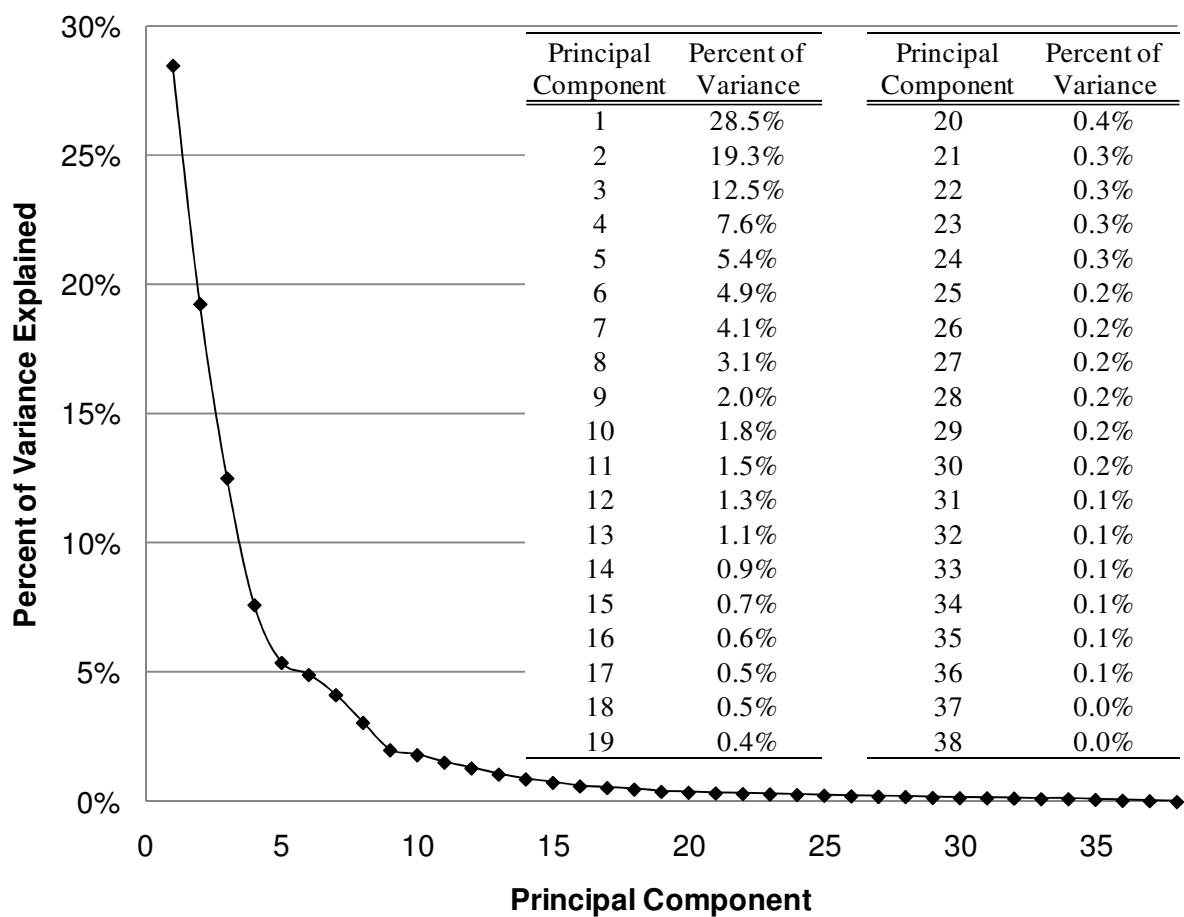


Figure S4: Plot showing the percentage of variance explained by each additional principal component. The table in the inset gives exact percentages for each PC.

Table S1: Physical and chemical properties measured for the water samples.

Site	Temperature (°C)	pH	Salinity	DOC (mg/L C) ^a
Wood Extract (WE)	-- ^b	5.0	0	89.42 ± 1.13
Dismal Swamp (DS)	25	3.2	0	92.74 ± 1.18
Great Bridge (GB)	29	7.6	18	7.45 ± 0.13
Town Point (TP)	29	7.7	24	3.34 ± 0.09
Chesapeake Bay Bridge (CBB)	28	7.9	30	2.15 ± 0.08
Offshore Coastal (OSC)	26	8.1	35	1.18 ± 0.04
Sta. 0	15	7.9	31	1.19 ± 0.16
Sta. 1	17	8.1	30	1.60 ± 0.21
Sta. 2	15	8.0	24	2.07 ± 0.20
Sta. 3	15	8.0	24	1.42 ± 0.08
Sta. 4	16	8.0	26	1.70 ± 0.26
Sta. 5	18	8.1	31	1.84 ± 0.24
Sta. 6	18	8.1	31	1.37 ± 0.33
Sta. 8	18	8.1	31	1.74 ± 0.18
Sta. 9	19	8.1	32	1.08 ± 0.22
Sta. 10	19	8.1	33	1.38 ± 0.07
Sta. 11	22	8.1	34	2.02 ± 0.06
Sta. 12- 2 m	21	8.1	35	0.97 ± 0.18
Sta. 12- 40 m	19	8.1	35	1.43 ± 0.13
Sta. 12- 200 m	10	8.1	35	2.19 ± 0.27
Sta. 12- 350 m	7	8.1	35	0.68 ± 0.16
Sta. 13- 2 m	19	8.1	33	1.06 ± 0.19
Sta. 13- 30 m	21	8.1	35	1.00 ± 0.10
Sta. 13- 401 m	7	8.1	35	0.42 ± 0.03
Sta. 14	18	8.1	34	1.41 ± 0.21
Sta. 15	17	8.1	32	1.01 ± 0.07

^a Error is the standard deviation of three measurements.^b The wood was extracted in water at room temperature.

Table S2: The number of peaks, number of assigned molecular formulas, and the percentage of peaks assigned a molecular formula for each sample.

Sample	Number of Peaks Assigned a Formula ^a	Percentage of Peaks Assigned a Formula
DS-WW, t=0	2517	92%
DS-WW, t=0	2619	92%
DS-WW, t=0	2581	92%
DS-WW, t=12 d	2403	95%
DS-WW, t=22 d	2310	90%
DS-WW, t=31 d	2462	94%
WE-WW	2300	86%
WE-C ₁₈	3028	88%
DS-C ₁₈	2901	94%
GB-C ₁₈	1563	84%
TP-C ₁₈	1291	92%
CBB-C ₁₈	1935	96%
OSC-C ₁₈	1480	85%
DS-ED	2911	99%
GB-ED	2027	76%
TP-ED	2868	99%
CBB-ED	2196	99%
OSC-ED	1256	85%
Sta 0	1700	93%
Sta 1	1636	95%
Sta 2	2091	99%
Sta 3	1506	94%
Sta 4	1260	98%
Sta 5	1695	96%
Sta 6	1853	98%
Sta 8	1723	95%
Sta 9	1711	97%
Sta 10	1257	93%
Sta 11	1525	95%
Sta 12, 2m	1409	93%
Sta 12, 40m	1586	98%
Sta 12, 200m	1495	99%
Sta 12, 350m	1251	92%
Sta 13, 2m	1205	91%
Sta 13, 30m	1201	92%
Sta 13, 401m	1225	96%
Sta 14	1680	95%
Sta 15	1467	93%

^a Excludes contributions from ¹³C isotopes

Table S3: Values of the bulk parameters used for HCA and PCA, before normalization. WW, C₁₈, and ED each indicate that the sample was analyzed as whole water, a C₁₈ extract, or after desalting by electrodialysis, respectively. All cruise station samples were C₁₈ extracted. The plots shown in Figure 1 were based on these parameters.

Sample	O/C _w	H/C _w	DBE _w	DBE/C _w	DBE/O _w	C# _w
DS-WW, t=0	0.33	1.20	9.28	0.45	1.49	20.15
DS-WW, t=0	0.33	1.23	9.10	0.44	1.47	20.17
DS-WW, t=0	0.33	1.21	9.28	0.45	1.47	20.17
DS-WW, t=12 d	0.33	1.19	9.15	0.46	1.52	19.55
DS-WW, t=22 d	0.34	1.17	9.31	0.47	1.50	19.53
DS-WW, t=31 d	0.33	1.20	9.08	0.46	1.46	19.43
WE-WW	0.41	1.21	8.50	0.45	1.19	18.65
WE-C ₁₈	0.29	1.19	9.35	0.46	1.75	20.02
DS-C ₁₈	0.32	1.18	10.22	0.46	1.60	22.48
GB-C ₁₈	0.34	1.30	8.43	0.40	1.20	21.03
TP-C ₁₈	0.34	1.38	8.19	0.36	1.16	21.52
CBB-C ₁₈	0.33	1.40	7.94	0.35	1.13	22.97
OSC-C ₁₈	0.34	1.41	7.60	0.34	1.03	21.98
DS-ED	0.48	1.10	10.60	0.50	1.14	21.22
GB-ED	0.48	1.21	10.11	0.50	0.91	20.45
TP-ED	0.43	1.46	6.71	0.33	0.83	20.06
CBB-ED	0.40	1.58	5.93	0.30	0.77	25.05
OSC-ED	0.40	1.61	5.10	0.26	0.75	19.10
Sta 0	0.27	1.50	6.62	0.30	1.22	21.83
Sta 1	0.28	1.46	7.05	0.32	1.29	22.22
Sta 2	0.26	1.45	6.76	0.33	1.48	20.60
Sta 3	0.29	1.44	7.46	0.33	1.32	22.40
Sta 4	0.28	1.45	6.77	0.33	1.22	20.80
Sta 5	0.27	1.46	6.74	0.32	1.37	20.49
Sta 6	0.24	1.50	6.27	0.30	1.45	20.26
Sta 8	0.27	1.43	7.63	0.33	1.48	22.76
Sta 9	0.26	1.46	6.74	0.32	1.43	20.76
Sta 10	0.29	1.46	6.94	0.32	1.17	21.44
Sta 11	0.30	1.44	7.56	0.33	1.21	22.99
Sta 12, 2m	0.30	1.43	7.76	0.33	1.26	23.12
Sta 12, 40m	0.30	1.45	7.45	0.32	1.21	22.76
Sta 12, 200m	0.33	1.41	8.00	0.34	1.16	23.00
Sta 12, 350m	0.32	1.42	7.99	0.33	1.26	23.67
Sta 13, 2m	0.31	1.44	6.97	0.33	1.14	21.10
Sta 13, 30m	0.31	1.45	6.89	0.32	1.11	21.17
Sta 13, 401m	0.31	1.45	7.06	0.33	1.08	21.40
Sta 14	0.29	1.43	7.65	0.33	1.31	22.93

Sta 15	0.29	1.44	7.57	0.33	1.30	22.84
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Table S4: Molecular formulas in the areas of the van Krevelen diagram shown in Figure 4. All formulas are of singly charged negative ions.

Area 1		Area 2		Area 3	
m/z	Formula	m/z	Formula	m/z	Formula
297.152989	C ₁₆ H ₂₅ O ₃ S ₁	247.173724	C ₁₃ H ₂₇ O ₂ S ₁	309.170747	C ₁₇ H ₂₅ O ₅
309.101347	C ₁₂ H ₂₁ O ₇ S ₁	279.127168	C ₁₂ H ₂₃ O ₅ S ₁	321.170747	C ₁₈ H ₂₅ O ₅
327.163554	C ₁₇ H ₂₇ O ₄ S ₁	281.142818	C ₁₂ H ₂₅ O ₅ S ₁	321.207133	C ₁₉ H ₂₉ O ₄
341.179204	C ₁₈ H ₂₉ O ₄ S ₁	283.137339	C ₁₅ H ₂₃ O ₃ S ₁	323.186398	C ₁₈ H ₂₇ O ₅
345.155491	C ₁₆ H ₂₅ O ₈	285.207133	C ₁₆ H ₂₉ O ₄	325.165662	C ₁₇ H ₂₅ O ₆
359.134756	C ₁₆ H ₂₃ O ₉	295.137339	C ₁₆ H ₂₃ O ₃ S ₁	325.202048	C ₁₈ H ₂₉ O ₅
365.163948	C ₁₆ H ₂₉ O ₇ S ₁	299.222783	C ₁₇ H ₃₁ O ₄	333.170747	C ₁₉ H ₂₅ O ₅
371.218760	C ₁₈ H ₃₁ N ₂ O ₆	313.096262	C ₁₁ H ₂₁ O ₈ S ₁	335.150012	C ₁₈ H ₂₃ O ₆
373.114020	C ₁₆ H ₂₁ O ₁₀	339.163554	C ₁₈ H ₂₇ O ₄ S ₁	335.186398	C ₁₉ H ₂₇ O ₅
373.150406	C ₁₇ H ₂₅ O ₉	341.108935	C ₁₂ H ₂₁ O ₁₁	335.222783	C ₂₀ H ₃₁ O ₄
383.134756	C ₁₈ H ₂₃ O ₉	341.306119	C ₂₁ H ₄₁ O ₃	337.165662	C ₁₈ H ₂₅ O ₆
385.150406	C ₁₈ H ₂₅ O ₉	343.139841	C ₁₆ H ₂₃ O ₈	337.202048	C ₁₉ H ₂₉ O ₅
387.129671	C ₁₇ H ₂₃ O ₁₀	347.134756	C ₁₅ H ₂₃ O ₉	337.238433	C ₂₀ H ₃₃ O ₄
387.166056	C ₁₈ H ₂₇ O ₉	353.179204	C ₁₉ H ₂₉ O ₄ S ₁	339.181312	C ₁₈ H ₂₇ O ₆
395.134756	C ₁₉ H ₂₃ O ₉	355.088200	C ₁₂ H ₁₉ O ₁₂	339.217698	C ₁₉ H ₃₁ O ₅
397.150406	C ₁₉ H ₂₅ O ₉	355.139841	C ₁₇ H ₂₃ O ₈	341.196962	C ₁₈ H ₂₉ O ₆
399.129671	C ₁₈ H ₂₃ O ₁₀	355.158468	C ₁₈ H ₂₇ O ₅ S ₁	347.150012	C ₁₉ H ₂₃ O ₆
399.166056	C ₁₉ H ₂₇ O ₉	355.285383	C ₂₁ H ₃₉ O ₄	347.186398	C ₂₀ H ₂₇ O ₅
401.108935	C ₁₇ H ₂₁ O ₁₁	357.103850	C ₁₂ H ₂₁ O ₁₂	347.222783	C ₂₁ H ₃₁ O ₄
401.145321	C ₁₈ H ₂₅ O ₁₀	357.137733	C ₁₇ H ₂₅ O ₆ S ₁	349.165662	C ₁₉ H ₂₅ O ₆
401.181706	C ₁₉ H ₂₉ O ₉	359.207527	C ₁₈ H ₃₁ O ₇	349.202048	C ₂₀ H ₂₉ O ₅
403.160971	C ₁₈ H ₂₇ O ₁₀	361.150406	C ₁₆ H ₂₅ O ₉	349.238433	C ₂₁ H ₃₃ O ₄
407.134756	C ₂₀ H ₂₃ O ₉	369.301033	C ₂₂ H ₄₁ O ₄	351.181312	C ₁₉ H ₂₇ O ₆
409.150406	C ₂₀ H ₂₅ O ₉	371.153383	C ₁₈ H ₂₇ O ₆ S ₁	353.160577	C ₁₈ H ₂₅ O ₇
411.129671	C ₁₉ H ₂₃ O ₁₀	375.166056	C ₁₇ H ₂₇ O ₉	353.196962	C ₁₉ H ₂₉ O ₆
411.166056	C ₂₀ H ₂₇ O ₉	377.145321	C ₁₆ H ₂₅ O ₁₀	355.176227	C ₁₈ H ₂₇ O ₇
413.145321	C ₁₉ H ₂₅ O ₁₀	379.114689	C ₁₇ H ₁₉ N ₂ O ₈	355.212612	C ₁₉ H ₃₁ O ₆
415.124585	C ₁₈ H ₂₃ O ₁₁	380.138461	C ₁₅ H ₂₆ N ₁ O ₈ S ₁	361.165662	C ₂₀ H ₂₅ O ₆
415.137472	C ₁₅ H ₂₈ O ₁₁ P ₁	393.176621	C ₁₇ H ₂₉ O ₁₀	361.202048	C ₂₁ H ₂₉ O ₅
415.160971	C ₁₉ H ₂₇ O ₁₀	396.142892	C ₁₅ H ₂₇ N ₁ O ₉ P ₁	361.238433	C ₂₂ H ₃₃ O ₄
417.176621	C ₁₉ H ₂₉ O ₁₀	396.179277	C ₁₆ H ₃₁ N ₁ O ₈ P ₁	363.181312	C ₂₀ H ₂₇ O ₆
417.213006	C ₂₀ H ₃₃ O ₉	397.135150	C ₁₅ H ₂₅ O ₁₂	363.217698	C ₂₁ H ₃₁ O ₅
421.150406	C ₂₁ H ₂₅ O ₉	399.142557	C ₁₅ H ₂₈ O ₁₀ P ₁	365.196962	C ₂₀ H ₂₉ O ₆
423.129671	C ₂₀ H ₂₃ O ₁₀	401.075920	C ₁₃ H ₂₁ O ₁₂ S ₁	365.233348	C ₂₁ H ₃₃ O ₅
425.145321	C ₂₀ H ₂₅ O ₁₀	403.197356	C ₁₉ H ₃₁ O ₉	367.176227	C ₁₉ H ₂₇ O ₇
429.140235	C ₁₉ H ₂₅ O ₁₁	405.070455	C ₁₄ H ₁₈ N ₂ O ₁₀ P ₁	367.212612	C ₂₀ H ₃₁ O ₆
429.176621	C ₂₀ H ₂₉ O ₁₀	405.176621	C ₁₈ H ₂₉ O ₁₀	369.191877	C ₁₉ H ₂₉ O ₇
431.155885	C ₁₉ H ₂₇ O ₁₁	407.192271	C ₁₈ H ₃₁ O ₁₀	373.202048	C ₂₂ H ₂₉ O ₅
431.192271	C ₂₀ H ₃₁ O ₁₀	408.169761	C ₁₇ H ₃₀ N ₁ O ₈ S ₁	375.181312	C ₂₁ H ₂₇ O ₆
436.161305	C ₂₁ H ₂₆ N ₁ O ₉	409.125254	C ₁₈ H ₂₁ N ₂ O ₉	375.217698	C ₂₂ H ₃₁ O ₅
437.145321	C ₂₁ H ₂₅ O ₁₀	409.171535	C ₁₇ H ₂₉ O ₁₁	377.196962	C ₂₁ H ₂₉ O ₆

439.160971	C ₂₁ H ₂₇ O ₁₀	410.194927	C ₁₇ H ₃₃ N ₁ O ₈ P ₁	377.233348	C ₂₂ H ₃₃ O ₅
441.140235	C ₂₀ H ₂₅ O ₁₁	415.145715	C ₁₅ H ₂₇ O ₁₃	379.176227	C ₂₀ H ₂₇ O ₇
443.155885	C ₂₀ H ₂₇ O ₁₁	419.192271	C ₁₉ H ₃₁ O ₁₀	379.212612	C ₂₁ H ₃₁ O ₆
443.192271	C ₂₁ H ₃₁ O ₁₀	421.171535	C ₁₈ H ₂₉ O ₁₁	379.248998	C ₂₂ H ₃₅ O ₅
445.171535	C ₂₀ H ₂₉ O ₁₁	423.187185	C ₁₈ H ₃₁ O ₁₁	381.191877	C ₂₀ H ₂₉ O ₇
449.145321	C ₂₂ H ₂₅ O ₁₀	424.161305	C ₂₀ H ₂₆ N ₁ O ₉	381.228262	C ₂₁ H ₃₃ O ₆
451.160971	C ₂₂ H ₂₇ O ₁₀	426.189842	C ₁₇ H ₃₃ N ₁ O ₉ P ₁	383.207527	C ₂₀ H ₃₁ O ₇
453.140235	C ₂₁ H ₂₅ O ₁₁	428.169106	C ₁₆ H ₃₁ N ₁ O ₁₀ P ₁	387.181312	C ₂₂ H ₂₇ O ₆
453.176621	C ₂₂ H ₂₉ O ₁₀	429.373804	C ₂₉ H ₄₉ O ₂	387.217698	C ₂₃ H ₃₁ O ₅
455.155885	C ₂₁ H ₂₇ O ₁₁	431.038486	C ₁₆ H ₁₆ O ₁₂ P ₁	389.196962	C ₂₂ H ₂₉ O ₆
457.135150	C ₂₀ H ₂₅ O ₁₂	431.140629	C ₁₅ H ₂₇ O ₁₄	389.233348	C ₂₃ H ₃₃ O ₅
457.171535	C ₂₁ H ₂₉ O ₁₁	431.168772	C ₁₆ H ₃₂ O ₁₁ P ₁	391.176227	C ₂₁ H ₂₇ O ₇
459.187185	C ₂₁ H ₃₁ O ₁₁	431.228656	C ₂₁ H ₃₅ O ₉	391.212612	C ₂₂ H ₃₁ O ₆
459.223571	C ₂₂ H ₃₅ O ₁₀	433.150406	C ₂₂ H ₂₅ O ₉	391.248998	C ₂₃ H ₃₅ O ₅
463.160971	C ₂₃ H ₂₇ O ₁₀	433.207921	C ₂₀ H ₃₃ O ₁₀	393.191877	C ₂₁ H ₂₉ O ₇
465.140235	C ₂₂ H ₂₅ O ₁₁	435.187185	C ₁₉ H ₃₁ O ₁₁	393.228262	C ₂₂ H ₃₃ O ₆
465.176621	C ₂₃ H ₂₉ O ₁₀	436.201061	C ₁₉ H ₃₄ N ₁ O ₈ S ₁	395.207527	C ₂₁ H ₃₁ O ₇
467.155885	C ₂₂ H ₂₇ O ₁₁	437.202835	C ₁₉ H ₃₃ O ₁₁	395.243912	C ₂₂ H ₃₅ O ₆
469.135150	C ₂₁ H ₂₅ O ₁₂	437.363634	C ₂₇ H ₄₉ O ₄	397.223177	C ₂₁ H ₃₃ O ₇
469.171535	C ₂₂ H ₂₉ O ₁₁	439.073812	C ₁₆ H ₂₃ O ₁₀ S ₂	401.196962	C ₂₃ H ₂₉ O ₆
471.150800	C ₂₁ H ₂₇ O ₁₂	439.193333	C ₁₇ H ₃₁ N ₂ O ₁₁	401.233348	C ₂₄ H ₃₃ O ₅
471.187185	C ₂₂ H ₃₁ O ₁₁	441.124979	C ₁₆ H ₂₅ O ₁₄	403.176227	C ₂₂ H ₂₇ O ₇
473.202835	C ₂₂ H ₃₃ O ₁₁	443.301427	C ₂₄ H ₄₃ O ₇	403.212612	C ₂₃ H ₃₁ O ₆
477.176621	C ₂₄ H ₂₉ O ₁₀	447.223571	C ₂₁ H ₃₅ O ₁₀	403.248998	C ₂₄ H ₃₅ O ₅
479.155885	C ₂₃ H ₂₇ O ₁₁	449.148691	C ₁₉ H ₂₉ O ₁₀ S ₁	405.191877	C ₂₂ H ₂₉ O ₇
481.171535	C ₂₃ H ₂₉ O ₁₁	449.169821	C ₁₆ H ₃₃ O ₁₂ S ₁	405.228262	C ₂₃ H ₃₃ O ₆
483.150800	C ₂₂ H ₂₇ O ₁₂	449.202835	C ₂₀ H ₃₃ O ₁₁	405.264648	C ₂₄ H ₃₇ O ₅
483.187185	C ₂₃ H ₃₁ O ₁₁	451.137472	C ₁₈ H ₂₈ O ₁₁ P ₁	407.207527	C ₂₂ H ₃₁ O ₇
485.166450	C ₂₂ H ₂₉ O ₁₂	452.205492	C ₁₉ H ₃₅ N ₁ O ₉ P ₁	407.243912	C ₂₃ H ₃₅ O ₆
485.202835	C ₂₃ H ₃₃ O ₁₁	455.101741	C ₂₀ H ₂₃ O ₁₀ S ₁	409.223177	C ₂₂ H ₃₃ O ₇
487.218486	C ₂₃ H ₃₅ O ₁₁	457.203898	C ₁₇ H ₃₃ N ₂ O ₁₂	409.259562	C ₂₃ H ₃₇ O ₆
493.171535	C ₂₄ H ₂₉ O ₁₁	457.317077	C ₂₅ H ₄₅ O ₇	415.212612	C ₂₄ H ₃₁ O ₆
495.150800	C ₂₃ H ₂₇ O ₁₂	461.042906	C ₁₄ H ₂₁ O ₁₃ S ₂	415.248998	C ₂₅ H ₃₅ O ₅
495.187185	C ₂₄ H ₃₁ O ₁₁	461.058162	C ₁₈ H ₂₁ O ₁₀ S ₂	417.191877	C ₂₃ H ₂₉ O ₇
497.166450	C ₂₃ H ₂₉ O ₁₂	461.202835	C ₂₁ H ₃₃ O ₁₁	417.228262	C ₂₄ H ₃₃ O ₆
497.202835	C ₂₄ H ₃₃ O ₁₁	461.363634	C ₂₉ H ₄₉ O ₄	417.264648	C ₂₅ H ₃₇ O ₅
499.182100	C ₂₃ H ₃₁ O ₁₂	463.218486	C ₂₁ H ₃₅ O ₁₁	419.207527	C ₂₃ H ₃₁ O ₇
499.218486	C ₂₄ H ₃₅ O ₁₁	463.342898	C ₂₈ H ₄₇ O ₅	419.243912	C ₂₄ H ₃₅ O ₆
505.171535	C ₂₅ H ₂₉ O ₁₁	464.205492	C ₂₀ H ₃₅ N ₁ O ₉ P ₁	419.280298	C ₂₅ H ₃₉ O ₅
507.187185	C ₂₅ H ₃₁ O ₁₁	465.197750	C ₂₀ H ₃₃ O ₁₂	421.223177	C ₂₃ H ₃₃ O ₇
509.166450	C ₂₄ H ₂₉ O ₁₂	465.394934	C ₂₉ H ₅₃ O ₄	421.259562	C ₂₄ H ₃₇ O ₆
511.182100	C ₂₄ H ₃₁ O ₁₂	466.221142	C ₂₀ H ₃₇ N ₁ O ₉ P ₁	423.238827	C ₂₃ H ₃₅ O ₇
513.161365	C ₂₃ H ₂₉ O ₁₃	467.159256	C ₁₉ H ₃₁ O ₁₁ S ₁	429.191877	C ₂₄ H ₂₉ O ₇
513.197750	C ₂₄ H ₃₃ O ₁₂	468.151134	C ₂₁ H ₂₆ N ₁ O ₁₁	429.228262	C ₂₅ H ₃₃ O ₆
515.213400	C ₂₄ H ₃₅ O ₁₂	470.151528	C ₁₇ H ₂₈ N ₁ O ₁₄	429.264648	C ₂₆ H ₃₇ O ₅
521.166450	C ₂₅ H ₂₉ O ₁₂	471.332727	C ₂₆ H ₄₇ O ₇	431.207527	C ₂₄ H ₃₁ O ₇
525.161365	C ₂₄ H ₂₉ O ₁₃	473.163948	C ₂₅ H ₂₉ O ₇ S ₁	431.243912	C ₂₅ H ₃₅ O ₆
525.197750	C ₂₅ H ₃₃ O ₁₂	475.160971	C ₂₄ H ₂₇ O ₁₀	431.280298	C ₂₆ H ₃₉ O ₅

527.177015	C ₂₄ H ₃₁ O ₁₃	475.182100	C ₂₁ H ₃₁ O ₁₂	433.223177	C ₂₄ H ₃₃ O ₇
527.213400	C ₂₅ H ₃₅ O ₁₂	475.218486	C ₂₂ H ₃₅ O ₁₁	433.259562	C ₂₅ H ₃₇ O ₆
529.229050	C ₂₅ H ₃₇ O ₁₂	477.197750	C ₂₁ H ₃₃ O ₁₂	435.238827	C ₂₄ H ₃₅ O ₇
535.182100	C ₂₆ H ₃₁ O ₁₂	477.358548	C ₂₉ H ₄₉ O ₅	435.275213	C ₂₅ H ₃₉ O ₆
537.197750	C ₂₆ H ₃₃ O ₁₂	479.205157	C ₂₁ H ₃₆ O ₁₀ P ₁	443.207527	C ₂₅ H ₃₁ O ₇
539.177015	C ₂₅ H ₃₁ O ₁₃	479.213400	C ₂₁ H ₃₅ O ₁₂	443.243912	C ₂₆ H ₃₅ O ₆
539.213400	C ₂₆ H ₃₅ O ₁₂	479.337813	C ₂₈ H ₄₇ O ₆	443.280298	C ₂₇ H ₃₉ O ₅
553.192665	C ₂₆ H ₃₃ O ₁₃	480.200406	C ₂₀ H ₃₅ N ₁ O ₁₀ P ₁	445.223177	C ₂₅ H ₃₃ O ₇
557.260350	C ₂₇ H ₄₁ O ₁₂	481.257193	C ₂₂ H ₄₂ O ₉ P ₁	445.259562	C ₂₆ H ₃₇ O ₆
		482.216057	C ₂₀ H ₃₇ N ₁ O ₁₀ P ₁	445.295948	C ₂₇ H ₄₁ O ₅
		483.135544	C ₁₈ H ₂₇ O ₁₅	447.238827	C ₂₅ H ₃₅ O ₇
		483.190556	C ₂₀ H ₃₅ O ₁₁ S ₁	447.275213	C ₂₆ H ₃₉ O ₆
		483.272843	C ₂₂ H ₄₄ O ₉ P ₁	449.254477	C ₂₅ H ₃₇ O ₇
		485.151194	C ₁₈ H ₂₉ O ₁₅	449.290863	C ₂₆ H ₄₁ O ₆
		485.348378	C ₂₇ H ₄₉ O ₇	451.233742	C ₂₄ H ₃₅ O ₈
		487.302490	C ₂₄ H ₄₃ N ₂ O ₈	451.270127	C ₂₅ H ₃₉ O ₇
		489.197750	C ₂₂ H ₃₃ O ₁₂	453.249392	C ₂₄ H ₃₇ O ₈
		491.213400	C ₂₂ H ₃₅ O ₁₂	457.223177	C ₂₆ H ₃₃ O ₇
		493.192665	C ₂₁ H ₃₃ O ₁₃	457.259562	C ₂₇ H ₃₇ O ₆
		493.196036	C ₁₈ H ₃₇ O ₁₃ S ₁	457.295948	C ₂₈ H ₄₁ O ₅
		494.216057	C ₂₁ H ₃₇ N ₁ O ₁₀ P ₁	459.238827	C ₂₆ H ₃₅ O ₇
		495.200072	C ₂₁ H ₃₆ O ₁₁ P ₁	459.275213	C ₂₇ H ₃₉ O ₆
		495.208315	C ₂₁ H ₃₅ O ₁₃	461.218092	C ₂₅ H ₃₃ O ₈
		496.195321	C ₂₀ H ₃₅ N ₁ O ₁₁ P ₁	461.254477	C ₂₆ H ₃₇ O ₇
		497.215722	C ₂₁ H ₃₈ O ₁₁ P ₁	461.290863	C ₂₇ H ₄₁ O ₆
		497.252108	C ₂₂ H ₄₂ O ₁₀ P ₁	463.233742	C ₂₅ H ₃₅ O ₈
		498.210971	C ₂₀ H ₃₇ N ₁ O ₁₁ P ₁	463.270127	C ₂₆ H ₃₉ O ₇
		499.364028	C ₂₈ H ₅₁ O ₇	463.306513	C ₂₇ H ₄₃ O ₆
		501.146108	C ₁₈ H ₂₉ O ₁₆	465.249392	C ₂₅ H ₃₇ O ₈
		503.213400	C ₂₃ H ₃₅ O ₁₂	471.275213	C ₂₈ H ₃₉ O ₆
		503.249786	C ₂₄ H ₃₉ O ₁₁	471.311598	C ₂₉ H ₄₃ O ₅
		505.159650	C ₁₈ H ₃₃ O ₁₄ S ₁	473.254477	C ₂₇ H ₃₇ O ₇
		505.192665	C ₂₂ H ₃₃ O ₁₃	473.290863	C ₂₈ H ₄₁ O ₆
		505.257193	C ₂₄ H ₄₂ O ₉ P ₁	475.233742	C ₂₆ H ₃₅ O ₈
		505.499005	C ₃₄ H ₆₅ O ₂	475.270127	C ₂₇ H ₃₉ O ₇
		507.205812	C ₂₆ H ₃₅ O ₈ S ₁	475.306513	C ₂₈ H ₄₃ O ₆
		507.208315	C ₂₂ H ₃₅ O ₁₃	477.249392	C ₂₆ H ₃₇ O ₈
		507.272843	C ₂₄ H ₄₄ O ₉ P ₁	477.285777	C ₂₇ H ₄₁ O ₇
		508.195321	C ₂₁ H ₃₅ N ₁ O ₁₁ P ₁	479.265042	C ₂₆ H ₃₉ O ₈
		508.231707	C ₂₂ H ₃₉ N ₁ O ₁₀ P ₁	479.301427	C ₂₇ H ₄₃ O ₇
		509.288493	C ₂₄ H ₄₆ O ₉ P ₁	481.280692	C ₂₆ H ₄₁ O ₈
		510.210971	C ₂₁ H ₃₇ N ₁ O ₁₁ P ₁	485.254477	C ₂₈ H ₃₇ O ₇
		512.162093	C ₁₉ H ₃₀ N ₁ O ₁₅	485.290863	C ₂₉ H ₄₁ O ₆
		513.247022	C ₂₂ H ₄₂ O ₁₁ P ₁	485.327248	C ₃₀ H ₄₅ O ₅
		517.141023	C ₁₈ H ₂₉ O ₁₇	487.270127	C ₂₈ H ₃₉ O ₇
		517.229050	C ₂₄ H ₃₇ O ₁₂	489.249392	C ₂₇ H ₃₇ O ₈
		519.187185	C ₂₆ H ₃₁ O ₁₁	489.285777	C ₂₈ H ₄₁ O ₇

519.208315	C ₂₃ H ₃₅ O ₁₃	491.265042	C ₂₇ H ₃₉ O ₈
519.244700	C ₂₄ H ₃₉ O ₁₂	491.301427	C ₂₈ H ₄₃ O ₇
520.231707	C ₂₃ H ₃₉ N ₁ O ₁₀ P ₁	493.280692	C ₂₇ H ₄₁ O ₈
521.187579	C ₂₂ H ₃₃ O ₁₄	495.296342	C ₂₇ H ₄₃ O ₈
521.223965	C ₂₃ H ₃₇ O ₁₃	499.270127	C ₂₉ H ₃₉ O ₇
521.252108	C ₂₄ H ₄₂ O ₁₀ P ₁	499.306513	C ₃₀ H ₄₃ O ₆
522.210971	C ₂₂ H ₃₇ N ₁ O ₁₁ P ₁	501.249392	C ₂₈ H ₃₇ O ₈
522.247357	C ₂₃ H ₄₁ N ₁ O ₁₀ P ₁	501.285777	C ₂₉ H ₄₁ O ₇
523.182100	C ₂₅ H ₃₁ O ₁₂	501.322163	C ₃₀ H ₄₅ O ₆
523.203229	C ₂₂ H ₃₅ O ₁₄	503.265042	C ₂₈ H ₃₉ O ₈
523.267758	C ₂₄ H ₄₄ O ₁₀ P ₁	503.301427	C ₂₉ H ₄₃ O ₇
524.226621	C ₂₂ H ₃₉ N ₁ O ₁₁ P ₁	503.337813	C ₃₀ H ₄₇ O ₆
525.146108	C ₂₀ H ₂₉ O ₁₆	505.244306	C ₂₇ H ₃₇ O ₉
525.283408	C ₂₄ H ₄₆ O ₁₀ P ₁	505.280692	C ₂₈ H ₄₁ O ₈
526.205886	C ₂₁ H ₃₇ N ₁ O ₁₂ P ₁	505.317077	C ₂₉ H ₄₅ O ₇
527.141498	C ₂₄ H ₃₁ O ₉ S ₂	505.353463	C ₃₀ H ₄₉ O ₆
527.299058	C ₂₄ H ₄₈ O ₁₀ P ₁	507.259956	C ₂₇ H ₃₉ O ₉
531.244700	C ₂₅ H ₃₉ O ₁₂	507.296342	C ₂₈ H ₄₃ O ₈
531.514655	C ₃₆ H ₆₇ O ₂	509.275606	C ₂₇ H ₄₁ O ₉
533.223965	C ₂₄ H ₃₇ O ₁₃	513.285777	C ₃₀ H ₄₁ O ₇
533.260350	C ₂₅ H ₄₁ O ₁₂	515.265042	C ₂₉ H ₃₉ O ₈
533.530305	C ₃₆ H ₆₉ O ₂	515.301427	C ₃₀ H ₄₃ O ₇
534.143940	C ₂₅ H ₂₈ N ₁ O ₁₀ S ₁	517.280692	C ₂₉ H ₄₁ O ₈
535.239615	C ₂₄ H ₃₉ O ₁₃	517.317077	C ₃₀ H ₄₅ O ₇
536.226621	C ₂₃ H ₃₉ N ₁ O ₁₁ P ₁	519.296342	C ₂₉ H ₄₃ O ₈
536.263007	C ₂₄ H ₄₃ N ₁ O ₁₀ P ₁	519.332727	C ₃₀ H ₄₇ O ₇
537.218879	C ₂₃ H ₃₇ O ₁₄	521.275606	C ₂₈ H ₄₁ O ₉
537.247022	C ₂₄ H ₄₂ O ₁₁ P ₁	521.311992	C ₂₉ H ₄₅ O ₈
537.255265	C ₂₄ H ₄₁ O ₁₃	523.291257	C ₂₈ H ₄₃ O ₉
538.242271	C ₂₃ H ₄₁ N ₁ O ₁₁ P ₁	529.280692	C ₃₀ H ₄₁ O ₈
539.138260	C ₁₇ H ₃₂ O ₁₇ P ₁	531.259956	C ₂₉ H ₃₉ O ₉
539.262672	C ₂₄ H ₄₄ O ₁₁ P ₁	531.296342	C ₃₀ H ₄₃ O ₈
540.221536	C ₂₂ H ₃₉ N ₁ O ₁₂ P ₁	533.275606	C ₂₉ H ₄₁ O ₉
541.278322	C ₂₄ H ₄₆ O ₁₁ P ₁	533.311992	C ₃₀ H ₄₅ O ₈
542.237186	C ₂₂ H ₄₁ N ₁ O ₁₂ P ₁	535.291257	C ₂₉ H ₄₃ O ₉
543.281086	C ₂₇ H ₄₃ O ₁₁	535.327642	C ₃₀ H ₄₇ O ₈
544.450020	C ₃₁ H ₆₃ N ₁ O ₄ P ₁	537.270521	C ₂₈ H ₄₁ O ₁₀
545.223965	C ₂₅ H ₃₇ O ₁₃	537.306907	C ₂₉ H ₄₅ O ₉
545.296736	C ₂₇ H ₄₅ O ₁₁	539.286171	C ₂₈ H ₄₃ O ₁₀
547.239615	C ₂₅ H ₃₉ O ₁₃	543.259956	C ₃₀ H ₃₉ O ₉
547.312386	C ₂₇ H ₄₇ O ₁₁	545.275606	C ₃₀ H ₄₁ O ₉
549.218879	C ₂₄ H ₃₇ O ₁₄	547.291257	C ₃₀ H ₄₃ O ₉
549.251242	C ₂₀ H ₄₁ N ₂ O ₁₅	549.270521	C ₂₉ H ₄₁ O ₁₀
549.255265	C ₂₅ H ₄₁ O ₁₃	549.306907	C ₃₀ H ₄₅ O ₉
550.242271	C ₂₄ H ₄₁ N ₁ O ₁₁ P ₁	551.286171	C ₂₉ H ₄₃ O ₁₀
551.226287	C ₂₄ H ₄₀ O ₁₂ P ₁	557.275606	C ₃₁ H ₄₁ O ₉
551.234530	C ₂₄ H ₃₉ O ₁₄	559.254871	C ₃₀ H ₃₉ O ₁₀

552.221536	C ₂₃ H ₃₉ N ₁ O ₁₂ P ₁	559.291257	C ₃₁ H ₄₃ O ₉
552.257921	C ₂₄ H ₄₃ N ₁ O ₁₁ P ₁	563.286171	C ₃₀ H ₄₃ O ₁₀
553.241937	C ₂₄ H ₄₂ O ₁₂ P ₁	565.265436	C ₂₉ H ₄₁ O ₁₁
553.250180	C ₂₄ H ₄₁ O ₁₄	565.301821	C ₃₀ H ₄₅ O ₁₀
554.237186	C ₂₃ H ₄₁ N ₁ O ₁₂ P ₁	573.270521	C ₃₁ H ₄₁ O ₁₀
555.229444	C ₂₃ H ₃₉ O ₁₅	575.286171	C ₃₁ H ₄₃ O ₁₀
555.257587	C ₂₄ H ₄₄ O ₁₂ P ₁	577.265436	C ₃₀ H ₄₁ O ₁₁
555.284457	C ₂₅ H ₄₇ O ₁₁ S ₁	579.281086	C ₃₀ H ₄₃ O ₁₁
556.252836	C ₂₃ H ₄₃ N ₁ O ₁₂ P ₁	587.286171	C ₃₂ H ₄₃ O ₁₀
557.273237	C ₂₄ H ₄₆ O ₁₂ P ₁	589.265436	C ₃₁ H ₄₁ O ₁₁
559.239615	C ₂₆ H ₃₉ O ₁₃	591.281086	C ₃₁ H ₄₃ O ₁₁
559.276000	C ₂₇ H ₄₃ O ₁₂	593.260350	C ₃₀ H ₄₁ O ₁₂
561.218879	C ₂₅ H ₃₇ O ₁₄	603.281086	C ₃₂ H ₄₃ O ₁₁
561.255265	C ₂₆ H ₄₁ O ₁₃		
561.291650	C ₂₇ H ₄₅ O ₁₂		
562.278657	C ₂₆ H ₄₅ N ₁ O ₁₀ P ₁		
563.234530	C ₂₅ H ₃₉ O ₁₄		
563.270915	C ₂₆ H ₄₃ O ₁₃		
563.307301	C ₂₇ H ₄₇ O ₁₂		
564.221536	C ₂₄ H ₃₉ N ₁ O ₁₂ P ₁		
565.213794	C ₂₄ H ₃₇ O ₁₅		
565.250180	C ₂₅ H ₄₁ O ₁₄		
565.322951	C ₂₇ H ₄₉ O ₁₂		
566.237186	C ₂₄ H ₄₁ N ₁ O ₁₂ P ₁		
566.273571	C ₂₅ H ₄₅ N ₁ O ₁₁ P ₁		
567.156673	C ₂₂ H ₃₁ O ₁₇		
567.229444	C ₂₄ H ₃₉ O ₁₅		
568.252836	C ₂₄ H ₄₃ N ₁ O ₁₂ P ₁		
569.236852	C ₂₄ H ₄₂ O ₁₃ P ₁		
569.241071	C ₁₉ H ₄₁ N ₂ O ₁₇		
569.245094	C ₂₄ H ₄₁ O ₁₅		
571.252502	C ₂₄ H ₄₄ O ₁₃ P ₁		
571.276000	C ₂₈ H ₄₃ O ₁₂		
571.288887	C ₂₅ H ₄₈ O ₁₂ P ₁		
573.255265	C ₂₇ H ₄₁ O ₁₃		
573.268152	C ₂₄ H ₄₆ O ₁₃ P ₁		
575.270915	C ₂₇ H ₄₃ O ₁₃		
575.435084	C ₃₂ H ₆₃ O ₆ S ₁		
577.250180	C ₂₆ H ₄₁ O ₁₄		
577.286565	C ₂₇ H ₄₅ O ₁₃		
579.229444	C ₂₅ H ₃₉ O ₁₅		
579.265830	C ₂₆ H ₄₃ O ₁₄		
579.302215	C ₂₇ H ₄₇ O ₁₃		
580.252836	C ₂₅ H ₄₃ N ₁ O ₁₂ P ₁		
580.289221	C ₂₆ H ₄₇ N ₁ O ₁₁ P ₁		
581.245094	C ₂₅ H ₄₁ O ₁₅		
582.232100	C ₂₄ H ₄₁ N ₁ O ₁₃ P ₁		

582.268486	C ₂₅ H ₄₅ N ₁ O ₁₂ P ₁
585.231766	C ₂₄ H ₄₂ O ₁₄ P ₁
585.240009	C ₂₄ H ₄₁ O ₁₆
587.247416	C ₂₄ H ₄₄ O ₁₄ P ₁
587.270915	C ₂₈ H ₄₃ O ₁₃
589.250180	C ₂₇ H ₄₁ O ₁₄
589.286565	C ₂₈ H ₄₅ O ₁₃
591.265830	C ₂₇ H ₄₃ O ₁₄
593.245094	C ₂₆ H ₄₁ O ₁₅
593.281480	C ₂₇ H ₄₅ O ₁₄
594.268486	C ₂₆ H ₄₅ N ₁ O ₁₂ P ₁
595.260744	C ₂₆ H ₄₃ O ₁₅
595.297130	C ₂₇ H ₄₇ O ₁₄
596.284136	C ₂₆ H ₄₇ N ₁ O ₁₂ P ₁
597.240009	C ₂₅ H ₄₁ O ₁₆
599.255659	C ₂₅ H ₄₃ O ₁₆
601.129277	C ₃₉ H ₂₁ O ₇
607.260744	C ₂₇ H ₄₃ O ₁₅
608.284136	C ₂₇ H ₄₇ N ₁ O ₁₂ P ₁
609.167238	C ₂₄ H ₃₃ O ₁₈
631.297130	C ₃₀ H ₄₇ O ₁₄
633.276394	C ₂₉ H ₄₅ O ₁₅
639.351487	C ₃₀ H ₅₆ O ₁₂ P ₁
645.276394	C ₃₀ H ₄₅ O ₁₅
647.292044	C ₃₀ H ₄₇ O ₁₅
657.261138	C ₂₇ H ₄₅ O ₁₈
661.416851	C ₃₄ H ₆₁ O ₁₂
664.672553	C ₄₂ H ₈₆ N ₃ O ₂
667.212612	C ₄₅ H ₃₁ O ₆
669.261138	C ₂₈ H ₄₅ O ₁₈
675.286959	C ₃₁ H ₄₇ O ₁₆
702.640584	C ₄₅ H ₈₄ N ₁ O ₄
709.292438	C ₃₁ H ₄₉ O ₁₈
711.308088	C ₃₁ H ₅₁ O ₁₈
718.614369	C ₄₈ H ₈₀ N ₁ O ₃
730.648385	C ₄₃ H ₈₉ N ₁ O ₅ P ₁

Area 4		Area 5		Area 6		Area 7	
m/z	Formula	m/z	Formula	m/z	Formula	m/z	Formula
233.118318	C ₁₄ H ₁₇ O ₃	233.045547	C ₁₂ H ₉ O ₅	285.061591	C ₁₂ H ₁₃ O ₈	359.061985	C ₁₄ H ₁₅ O ₁₁
235.097583	C ₁₃ H ₁₅ O ₄	237.076847	C ₁₂ H ₁₃ O ₅	287.077241	C ₁₂ H ₁₅ O ₈	371.025599	C ₁₄ H ₁₁ O ₁₂
235.133968	C ₁₄ H ₁₉ O ₃	241.050632	C ₁₄ H ₉ O ₄	297.061591	C ₁₃ H ₁₃ O ₈	371.061985	C ₁₅ H ₁₅ O ₁₁
243.139053	C ₁₆ H ₁₉ O ₂	243.066282	C ₁₄ H ₁₁ O ₄	299.077241	C ₁₃ H ₁₅ O ₈	373.041249	C ₁₄ H ₁₃ O ₁₂
245.118318	C ₁₅ H ₁₇ O ₃	245.045547	C ₁₃ H ₉ O ₅	301.056506	C ₁₂ H ₁₃ O ₉	373.077635	C ₁₅ H ₁₇ O ₁₁
245.154703	C ₁₆ H ₂₁ O ₂	245.081932	C ₁₄ H ₁₃ O ₄	301.092891	C ₁₃ H ₁₇ O ₈	375.056900	C ₁₄ H ₁₅ O ₁₂
247.097583	C ₁₄ H ₁₅ O ₄	247.061197	C ₁₃ H ₁₁ O ₅	309.061591	C ₁₄ H ₁₃ O ₈	383.025599	C ₁₅ H ₁₁ O ₁₂

249.113233	C ₁₄ H ₁₇ O ₄	249.040462	C ₁₂ H ₉ O ₆	311.040856	C ₁₃ H ₁₁ O ₉	385.041249	C ₁₅ H ₁₃ O ₁₂
255.139053	C ₁₇ H ₁₉ O ₂	249.076847	C ₁₃ H ₁₃ O ₅	311.077241	C ₁₄ H ₁₅ O ₈	385.077635	C ₁₆ H ₁₇ O ₁₁
257.118318	C ₁₆ H ₁₇ O ₃	251.056112	C ₁₂ H ₁₁ O ₆	313.056506	C ₁₃ H ₁₃ O ₉	387.020514	C ₁₄ H ₁₁ O ₁₃
257.154703	C ₁₇ H ₂₁ O ₂	253.050632	C ₁₅ H ₉ O ₄	313.092891	C ₁₄ H ₁₇ O ₈	387.056900	C ₁₅ H ₁₅ O ₁₂
259.097583	C ₁₅ H ₁₅ O ₄	255.066282	C ₁₅ H ₁₁ O ₄	315.072156	C ₁₃ H ₁₅ O ₉	389.036164	C ₁₄ H ₁₃ O ₁₃
259.133968	C ₁₆ H ₁₉ O ₃	257.045547	C ₁₄ H ₉ O ₅	321.061591	C ₁₅ H ₁₃ O ₈	389.072550	C ₁₅ H ₁₇ O ₁₂
259.170354	C ₁₇ H ₂₃ O ₂	257.081932	C ₁₅ H ₁₃ O ₄	323.040856	C ₁₄ H ₁₁ O ₉	395.025599	C ₁₆ H ₁₁ O ₁₂
261.149618	C ₁₆ H ₂₁ O ₃	259.061197	C ₁₄ H ₁₁ O ₅	323.077241	C ₁₅ H ₁₅ O ₈	397.041249	C ₁₆ H ₁₃ O ₁₂
263.092497	C ₁₄ H ₁₅ O ₅	261.040462	C ₁₃ H ₉ O ₆	325.056506	C ₁₄ H ₁₃ O ₉	397.077635	C ₁₇ H ₁₇ O ₁₁
267.139053	C ₁₈ H ₁₉ O ₂	261.076847	C ₁₄ H ₁₃ O ₅	325.092891	C ₁₅ H ₁₇ O ₈	399.020514	C ₁₅ H ₁₁ O ₁₃
269.081932	C ₁₆ H ₁₃ O ₄	263.056112	C ₁₃ H ₁₁ O ₆	327.035770	C ₁₃ H ₁₁ O ₁₀	399.056900	C ₁₆ H ₁₅ O ₁₂
269.118318	C ₁₇ H ₁₇ O ₃	265.035376	C ₁₂ H ₉ O ₇	327.072156	C ₁₄ H ₁₅ O ₉	401.036164	C ₁₅ H ₁₃ O ₁₃
269.154703	C ₁₈ H ₂₁ O ₂	265.050632	C ₁₆ H ₉ O ₄	329.051420	C ₁₃ H ₁₃ O ₁₀	401.072550	C ₁₆ H ₁₇ O ₁₂
271.097583	C ₁₆ H ₁₅ O ₄	265.071762	C ₁₃ H ₁₃ O ₆	329.087806	C ₁₄ H ₁₇ O ₉	403.051814	C ₁₅ H ₁₅ O ₁₃
271.133968	C ₁₇ H ₁₉ O ₃	267.051026	C ₁₂ H ₁₁ O ₇	335.040856	C ₁₅ H ₁₁ O ₉	409.041249	C ₁₇ H ₁₃ O ₁₂
271.170354	C ₁₈ H ₂₃ O ₂	267.066282	C ₁₆ H ₁₁ O ₄	335.077241	C ₁₆ H ₁₅ O ₈	411.020514	C ₁₆ H ₁₁ O ₁₃
273.113233	C ₁₆ H ₁₇ O ₄	269.045547	C ₁₅ H ₉ O ₅	337.056506	C ₁₅ H ₁₃ O ₉	411.056900	C ₁₇ H ₁₅ O ₁₂
273.149618	C ₁₇ H ₂₁ O ₃	271.061197	C ₁₅ H ₁₁ O ₅	337.092891	C ₁₆ H ₁₇ O ₈	413.036164	C ₁₆ H ₁₃ O ₁₃
273.186004	C ₁₈ H ₂₅ O ₂	273.040462	C ₁₄ H ₉ O ₆	339.035770	C ₁₄ H ₁₁ O ₁₀	413.072550	C ₁₇ H ₁₇ O ₁₂
275.092497	C ₁₅ H ₁₅ O ₅	273.076847	C ₁₅ H ₁₃ O ₅	339.072156	C ₁₅ H ₁₅ O ₉	415.015429	C ₁₅ H ₁₁ O ₁₄
275.128883	C ₁₆ H ₁₉ O ₄	275.056112	C ₁₄ H ₁₁ O ₆	339.108541	C ₁₆ H ₁₉ O ₈	415.051814	C ₁₆ H ₁₅ O ₁₃
281.118318	C ₁₈ H ₁₇ O ₃	277.035376	C ₁₃ H ₉ O ₇	341.051420	C ₁₄ H ₁₃ O ₁₀	415.088200	C ₁₇ H ₁₉ O ₁₂
281.154703	C ₁₉ H ₂₁ O ₂	277.071762	C ₁₄ H ₁₃ O ₆	341.087806	C ₁₅ H ₁₇ O ₉	417.031079	C ₁₅ H ₁₃ O ₁₄
283.097583	C ₁₇ H ₁₅ O ₄	279.051026	C ₁₃ H ₁₁ O ₇	343.030685	C ₁₃ H ₁₁ O ₁₁	417.067464	C ₁₆ H ₁₇ O ₁₃
283.133968	C ₁₈ H ₁₉ O ₃	279.066282	C ₁₇ H ₁₁ O ₄	343.067070	C ₁₄ H ₁₅ O ₁₀	417.103850	C ₁₇ H ₂₁ O ₁₂
283.170354	C ₁₉ H ₂₃ O ₂	281.045547	C ₁₆ H ₉ O ₅	343.103456	C ₁₅ H ₁₉ O ₉	421.041249	C ₁₈ H ₁₃ O ₁₂
285.113233	C ₁₇ H ₁₇ O ₄	281.066676	C ₁₃ H ₁₃ O ₇	347.040856	C ₁₆ H ₁₁ O ₉	423.020514	C ₁₇ H ₁₁ O ₁₃
285.149618	C ₁₈ H ₂₁ O ₃	281.081932	C ₁₇ H ₁₃ O ₄	349.056506	C ₁₆ H ₁₃ O ₉	425.036164	C ₁₇ H ₁₃ O ₁₃
287.092497	C ₁₆ H ₁₅ O ₅	283.061197	C ₁₆ H ₁₁ O ₅	349.092891	C ₁₇ H ₁₇ O ₈	425.072550	C ₁₈ H ₁₇ O ₁₂
287.128883	C ₁₇ H ₁₉ O ₄	285.040462	C ₁₅ H ₉ O ₆	351.035770	C ₁₅ H ₁₁ O ₁₀	427.051814	C ₁₇ H ₁₅ O ₁₃
287.165268	C ₁₈ H ₂₃ O ₃	285.076847	C ₁₆ H ₁₃ O ₅	351.072156	C ₁₆ H ₁₅ O ₉	429.031079	C ₁₆ H ₁₃ O ₁₄
289.108147	C ₁₆ H ₁₇ O ₅	287.056112	C ₁₅ H ₁₁ O ₆	351.108541	C ₁₇ H ₁₉ O ₈	429.067464	C ₁₇ H ₁₇ O ₁₃
289.144533	C ₁₇ H ₂₁ O ₄	289.035376	C ₁₄ H ₉ O ₇	353.051420	C ₁₅ H ₁₃ O ₁₀	431.046729	C ₁₆ H ₁₅ O ₁₄
291.123797	C ₁₆ H ₁₉ O ₅	289.071762	C ₁₅ H ₁₃ O ₆	353.087806	C ₁₆ H ₁₇ O ₉	431.083114	C ₁₇ H ₁₉ O ₁₃
293.154703	C ₂₀ H ₂₁ O ₂	291.051026	C ₁₄ H ₁₁ O ₇	355.030685	C ₁₄ H ₁₁ O ₁₁	433.062379	C ₁₆ H ₁₇ O ₁₄
295.097583	C ₁₈ H ₁₅ O ₄	291.066282	C ₁₈ H ₁₁ O ₄	355.067070	C ₁₅ H ₁₅ O ₁₀	437.036164	C ₁₈ H ₁₃ O ₁₃
295.133968	C ₁₉ H ₁₉ O ₃	291.087412	C ₁₅ H ₁₅ O ₆	357.046335	C ₁₄ H ₁₃ O ₁₁	437.072550	C ₁₉ H ₁₇ O ₁₂
295.170354	C ₂₀ H ₂₃ O ₂	293.030291	C ₁₃ H ₉ O ₈	361.056506	C ₁₇ H ₁₃ O ₉	439.051814	C ₁₈ H ₁₅ O ₁₃
297.113233	C ₁₈ H ₁₇ O ₄	293.045547	C ₁₇ H ₉ O ₅	363.072156	C ₁₇ H ₁₅ O ₉	439.088200	C ₁₉ H ₁₉ O ₁₂
297.149618	C ₁₉ H ₂₁ O ₃	293.066676	C ₁₄ H ₁₃ O ₇	363.108541	C ₁₈ H ₁₉ O ₈	441.031079	C ₁₇ H ₁₃ O ₁₄
297.186004	C ₂₀ H ₂₅ O ₂	293.081932	C ₁₈ H ₁₃ O ₄	365.051420	C ₁₆ H ₁₃ O ₁₀	441.067464	C ₁₈ H ₁₇ O ₁₃
299.092497	C ₁₇ H ₁₅ O ₅	295.045941	C ₁₃ H ₁₁ O ₈	365.087806	C ₁₇ H ₁₇ O ₉	443.046729	C ₁₇ H ₁₅ O ₁₄
299.128883	C ₁₈ H ₁₉ O ₄	295.061197	C ₁₇ H ₁₁ O ₅	367.030685	C ₁₅ H ₁₁ O ₁₁	443.083114	C ₁₈ H ₁₉ O ₁₃
299.165268	C ₁₉ H ₂₃ O ₃	297.040462	C ₁₆ H ₉ O ₆	367.067070	C ₁₆ H ₁₅ O ₁₀	445.062379	C ₁₇ H ₁₇ O ₁₄
301.108147	C ₁₇ H ₁₇ O ₅	297.076847	C ₁₇ H ₁₃ O ₅	369.046335	C ₁₅ H ₁₃ O ₁₁	447.129671	C ₂₂ H ₂₃ O ₁₀
301.144533	C ₁₈ H ₂₁ O ₄	299.056112	C ₁₆ H ₁₁ O ₆	373.056506	C ₁₈ H ₁₃ O ₉	449.036164	C ₁₉ H ₁₃ O ₁₃
303.123797	C ₁₇ H ₁₉ O ₅	301.035376	C ₁₅ H ₉ O ₇	375.072156	C ₁₈ H ₁₅ O ₉	449.072550	C ₂₀ H ₁₇ O ₁₂
305.139447	C ₁₇ H ₂₁ O ₅	301.071762	C ₁₆ H ₁₃ O ₆	375.108541	C ₁₉ H ₁₉ O ₈	451.051814	C ₁₉ H ₁₅ O ₁₃

307.097583	C ₁₉ H ₁₅ O ₄	303.051026	C ₁₅ H ₁₁ O ₇	377.051420	C ₁₇ H ₁₃ O ₁₀	451.088200	C ₂₀ H ₁₉ O ₁₂
307.133968	C ₂₀ H ₁₉ O ₃	303.087412	C ₁₆ H ₁₅ O ₆	377.087806	C ₁₈ H ₁₇ O ₉	453.031079	C ₁₈ H ₁₃ O ₁₄
309.113233	C ₁₉ H ₁₇ O ₄	305.030291	C ₁₄ H ₉ O ₈	379.030685	C ₁₆ H ₁₁ O ₁₁	453.067464	C ₁₉ H ₁₇ O ₁₃
309.149618	C ₂₀ H ₂₁ O ₃	305.045547	C ₁₈ H ₉ O ₅	379.067070	C ₁₇ H ₁₅ O ₁₀	453.103850	C ₂₀ H ₂₁ O ₁₂
309.186004	C ₂₁ H ₂₅ O ₂	305.066676	C ₁₅ H ₁₃ O ₇	379.103456	C ₁₈ H ₁₉ O ₉	455.046729	C ₁₈ H ₁₅ O ₁₄
311.128883	C ₁₉ H ₁₉ O ₄	305.081932	C ₁₉ H ₁₃ O ₄	381.046335	C ₁₆ H ₁₃ O ₁₁	455.083114	C ₁₉ H ₁₉ O ₁₃
311.165268	C ₂₀ H ₂₃ O ₃	305.103062	C ₁₆ H ₁₇ O ₆	381.082720	C ₁₇ H ₁₇ O ₁₀	457.062379	C ₁₈ H ₁₇ O ₁₄
311.201654	C ₂₁ H ₂₇ O ₂	307.045941	C ₁₄ H ₁₁ O ₈	387.072156	C ₁₉ H ₁₅ O ₉	457.098764	C ₁₉ H ₂₁ O ₁₃
313.108147	C ₁₈ H ₁₇ O ₅	307.061197	C ₁₈ H ₁₁ O ₅	389.051420	C ₁₈ H ₁₃ O ₁₀	459.041643	C ₁₇ H ₁₅ O ₁₅
313.144533	C ₁₉ H ₂₁ O ₄	309.040462	C ₁₇ H ₉ O ₆	389.087806	C ₁₉ H ₁₇ O ₉	465.031079	C ₁₉ H ₁₃ O ₁₄
313.180918	C ₂₀ H ₂₅ O ₃	309.076847	C ₁₈ H ₁₃ O ₅	391.030685	C ₁₇ H ₁₁ O ₁₁	465.067464	C ₂₀ H ₁₇ O ₁₃
315.123797	C ₁₈ H ₁₉ O ₅	311.056112	C ₁₇ H ₁₁ O ₆	391.067070	C ₁₈ H ₁₅ O ₁₀	467.046729	C ₁₉ H ₁₅ O ₁₄
315.160183	C ₁₉ H ₂₃ O ₄	313.035376	C ₁₆ H ₉ O ₇	391.103456	C ₁₉ H ₁₉ O ₉	467.083114	C ₂₀ H ₁₉ O ₁₃
317.139447	C ₁₈ H ₂₁ O ₅	313.071762	C ₁₇ H ₁₃ O ₆	393.046335	C ₁₇ H ₁₃ O ₁₁	469.025993	C ₁₈ H ₁₃ O ₁₅
319.118712	C ₁₇ H ₁₉ O ₆	315.051026	C ₁₆ H ₁₁ O ₇	393.082720	C ₁₈ H ₁₇ O ₁₀	469.062379	C ₁₉ H ₁₇ O ₁₄
321.113233	C ₂₀ H ₁₇ O ₄	317.030291	C ₁₅ H ₉ O ₈	395.061985	C ₁₇ H ₁₅ O ₁₁	469.098764	C ₂₀ H ₂₁ O ₁₃
321.149618	C ₂₁ H ₂₁ O ₃	317.066676	C ₁₆ H ₁₃ O ₇	399.072156	C ₂₀ H ₁₅ O ₉	471.078029	C ₁₉ H ₁₉ O ₁₄
321.186004	C ₂₂ H ₂₅ O ₂	317.103062	C ₁₇ H ₁₇ O ₆	401.051420	C ₁₉ H ₁₃ O ₁₀	473.057293	C ₁₈ H ₁₇ O ₁₅
323.128883	C ₂₀ H ₁₉ O ₄	319.045941	C ₁₅ H ₁₁ O ₈	401.087806	C ₂₀ H ₁₇ O ₉	473.093679	C ₁₉ H ₂₁ O ₁₄
323.165268	C ₂₁ H ₂₃ O ₃	319.061197	C ₁₉ H ₁₁ O ₅	403.067070	C ₁₉ H ₁₅ O ₁₀	477.031079	C ₂₀ H ₁₃ O ₁₄
323.201654	C ₂₂ H ₂₇ O ₂	319.082326	C ₁₆ H ₁₅ O ₇	403.103456	C ₂₀ H ₁₉ O ₉	477.103850	C ₂₂ H ₂₁ O ₁₂
325.108147	C ₁₉ H ₁₇ O ₅	319.097583	C ₂₀ H ₁₅ O ₄	405.046335	C ₁₈ H ₁₃ O ₁₁	479.046729	C ₂₀ H ₁₅ O ₁₄
325.144533	C ₂₀ H ₂₁ O ₄	321.040462	C ₁₈ H ₉ O ₆	405.082720	C ₁₉ H ₁₇ O ₁₀	479.083114	C ₂₁ H ₁₉ O ₁₃
325.180918	C ₂₁ H ₂₅ O ₃	321.076847	C ₁₉ H ₁₃ O ₅	407.061985	C ₁₈ H ₁₅ O ₁₁	481.025993	C ₁₉ H ₁₃ O ₁₅
327.123797	C ₁₉ H ₁₉ O ₅	323.056112	C ₁₈ H ₁₁ O ₆	407.098370	C ₁₉ H ₁₉ O ₁₀	481.062379	C ₂₀ H ₁₇ O ₁₄
327.160183	C ₂₀ H ₂₃ O ₄	323.092497	C ₁₉ H ₁₅ O ₅	413.087806	C ₂₁ H ₁₇ O ₉	481.098764	C ₂₁ H ₂₁ O ₁₃
327.196568	C ₂₁ H ₂₇ O ₃	325.035376	C ₁₇ H ₉ O ₇	415.067070	C ₂₀ H ₁₅ O ₁₀	483.041643	C ₁₉ H ₁₅ O ₁₅
329.103062	C ₁₈ H ₁₇ O ₆	325.071762	C ₁₈ H ₁₃ O ₆	415.103456	C ₂₁ H ₁₉ O ₉	483.078029	C ₂₀ H ₁₉ O ₁₄
329.139447	C ₁₉ H ₂₁ O ₅	327.051026	C ₁₇ H ₁₁ O ₇	417.046335	C ₁₉ H ₁₃ O ₁₁	483.114414	C ₂₁ H ₂₃ O ₁₃
331.118712	C ₁₈ H ₁₉ O ₆	329.030291	C ₁₆ H ₉ O ₈	417.082720	C ₂₀ H ₁₇ O ₁₀	485.057293	C ₁₉ H ₁₇ O ₁₅
335.128883	C ₂₁ H ₁₉ O ₄	329.066676	C ₁₇ H ₁₃ O ₇	417.119106	C ₂₁ H ₂₁ O ₉	485.093679	C ₂₀ H ₂₁ O ₁₄
335.165268	C ₂₂ H ₂₃ O ₃	331.045941	C ₁₆ H ₁₁ O ₈	419.061985	C ₁₉ H ₁₅ O ₁₁	491.046729	C ₂₁ H ₁₅ O ₁₄
335.201654	C ₂₃ H ₂₇ O ₂	331.061197	C ₂₀ H ₁₁ O ₅	419.098370	C ₂₀ H ₁₉ O ₁₀	491.083114	C ₂₂ H ₁₉ O ₁₃
337.108147	C ₂₀ H ₁₇ O ₅	333.040462	C ₁₉ H ₉ O ₆	421.077635	C ₁₉ H ₁₇ O ₁₁	493.062379	C ₂₁ H ₁₇ O ₁₄
337.144533	C ₂₁ H ₂₁ O ₄	333.076847	C ₂₀ H ₁₃ O ₅	427.067070	C ₂₁ H ₁₅ O ₁₀	493.098764	C ₂₂ H ₂₁ O ₁₃
337.180918	C ₂₂ H ₂₅ O ₃	333.097976	C ₁₇ H ₁₇ O ₇	427.103456	C ₂₂ H ₁₉ O ₉	495.078029	C ₂₁ H ₁₉ O ₁₄
339.123797	C ₂₀ H ₁₉ O ₅	333.113233	C ₂₁ H ₁₇ O ₄	429.082720	C ₂₁ H ₁₇ O ₁₀	495.114414	C ₂₂ H ₂₃ O ₁₃
339.160183	C ₂₁ H ₂₃ O ₄	335.056112	C ₁₉ H ₁₁ O ₆	429.119106	C ₂₂ H ₂₁ O ₉	497.057293	C ₂₀ H ₁₇ O ₁₅
339.196568	C ₂₂ H ₂₇ O ₃	335.092497	C ₂₀ H ₁₅ O ₅	431.061985	C ₂₀ H ₁₅ O ₁₁	497.093679	C ₂₁ H ₂₁ O ₁₄
341.103062	C ₁₉ H ₁₇ O ₆	337.035376	C ₁₈ H ₉ O ₇	431.098370	C ₂₁ H ₁₉ O ₁₀	503.046729	C ₂₂ H ₁₅ O ₁₄
341.139447	C ₂₀ H ₂₁ O ₅	337.071762	C ₁₉ H ₁₃ O ₆	433.041249	C ₁₉ H ₁₃ O ₁₂	503.155885	C ₂₅ H ₂₇ O ₁₁
341.175833	C ₂₁ H ₂₅ O ₄	339.051026	C ₁₈ H ₁₁ O ₇	433.077635	C ₂₀ H ₁₇ O ₁₁	505.135150	C ₂₄ H ₂₅ O ₁₂
341.212218	C ₂₂ H ₂₉ O ₃	341.030291	C ₁₇ H ₉ O ₈	433.114020	C ₂₁ H ₂₁ O ₁₀	507.041643	C ₂₁ H ₁₅ O ₁₅
343.118712	C ₁₉ H ₁₉ O ₆	341.066676	C ₁₈ H ₁₃ O ₇	435.056900	C ₁₉ H ₁₅ O ₁₂	507.078029	C ₂₂ H ₁₉ O ₁₄
343.155097	C ₂₀ H ₂₃ O ₅	343.045941	C ₁₇ H ₁₁ O ₈	435.093285	C ₂₀ H ₁₉ O ₁₁	507.114414	C ₂₃ H ₂₃ O ₁₃
345.134362	C ₁₉ H ₂₁ O ₆	343.082326	C ₁₈ H ₁₅ O ₇	441.082720	C ₂₂ H ₁₇ O ₁₀	509.057293	C ₂₁ H ₁₇ O ₁₅
349.144533	C ₂₂ H ₂₁ O ₄	345.025205	C ₁₆ H ₉ O ₉	441.119106	C ₂₃ H ₂₁ O ₉	509.093679	C ₂₂ H ₂₁ O ₁₄

349.180918	C ₂₃ H ₂₅ O ₃	345.061591	C ₁₇ H ₁₃ O ₈	443.098370	C ₂₂ H ₁₉ O ₁₀	509.130064	C ₂₃ H ₂₅ O ₁₃
351.123797	C ₂₁ H ₁₉ O ₅	345.097976	C ₁₈ H ₁₇ O ₇	445.041249	C ₂₀ H ₁₃ O ₁₂	511.036558	C ₂₀ H ₁₅ O ₁₆
351.160183	C ₂₂ H ₂₃ O ₄	347.056112	C ₂₀ H ₁₁ O ₆	445.077635	C ₂₁ H ₁₇ O ₁₁	511.072944	C ₂₁ H ₁₉ O ₁₅
351.196568	C ₂₃ H ₂₇ O ₃	347.077241	C ₁₇ H ₁₅ O ₈	447.056900	C ₂₀ H ₁₅ O ₁₂	513.088594	C ₂₁ H ₂₁ O ₁₅
353.139447	C ₂₁ H ₂₁ O ₅	347.092497	C ₂₁ H ₁₅ O ₅	447.093285	C ₂₁ H ₁₉ O ₁₁	517.062379	C ₂₃ H ₁₇ O ₁₄
353.175833	C ₂₂ H ₂₅ O ₄	349.035376	C ₁₉ H ₉ O ₇	453.119106	C ₂₄ H ₂₁ O ₉	519.041643	C ₂₂ H ₁₅ O ₁₅
353.212218	C ₂₃ H ₂₉ O ₃	349.071762	C ₂₀ H ₁₃ O ₆	455.098370	C ₂₃ H ₁₉ O ₁₀	519.078029	C ₂₃ H ₁₉ O ₁₄
355.118712	C ₂₀ H ₁₉ O ₆	349.108147	C ₂₁ H ₁₇ O ₅	455.134756	C ₂₄ H ₂₃ O ₉	519.114414	C ₂₄ H ₂₃ O ₁₃
355.155097	C ₂₁ H ₂₃ O ₅	351.051026	C ₁₉ H ₁₁ O ₇	457.077635	C ₂₂ H ₁₇ O ₁₁	519.150800	C ₂₅ H ₂₇ O ₁₂
355.191483	C ₂₂ H ₂₇ O ₄	351.087412	C ₂₀ H ₁₅ O ₆	457.114020	C ₂₃ H ₂₁ O ₁₀	521.057293	C ₂₂ H ₁₇ O ₁₅
357.134362	C ₂₀ H ₂₁ O ₆	353.030291	C ₁₈ H ₉ O ₈	459.056900	C ₂₁ H ₁₅ O ₁₂	521.093679	C ₂₃ H ₂₁ O ₁₄
357.170747	C ₂₁ H ₂₅ O ₅	353.066676	C ₁₉ H ₁₃ O ₇	459.093285	C ₂₂ H ₁₉ O ₁₁	521.130064	C ₂₄ H ₂₅ O ₁₃
363.160183	C ₂₃ H ₂₃ O ₄	353.103062	C ₂₀ H ₁₇ O ₆	461.072550	C ₂₁ H ₁₇ O ₁₂	523.036558	C ₂₁ H ₁₅ O ₁₆
365.139447	C ₂₂ H ₂₁ O ₅	355.045941	C ₁₈ H ₁₁ O ₈	461.108935	C ₂₂ H ₂₁ O ₁₁	523.072944	C ₂₂ H ₁₉ O ₁₅
365.175833	C ₂₃ H ₂₅ O ₄	355.082326	C ₁₉ H ₁₅ O ₇	463.088200	C ₂₁ H ₁₉ O ₁₂	523.109329	C ₂₃ H ₂₃ O ₁₄
365.212218	C ₂₄ H ₂₉ O ₃	357.025205	C ₁₇ H ₉ O ₉	469.114020	C ₂₄ H ₂₁ O ₁₀	523.145715	C ₂₄ H ₂₇ O ₁₃
367.155097	C ₂₂ H ₂₃ O ₅	357.061591	C ₁₈ H ₁₃ O ₈	469.150406	C ₂₅ H ₂₅ O ₉	525.052208	C ₂₁ H ₁₇ O ₁₆
367.191483	C ₂₃ H ₂₇ O ₄	357.097976	C ₁₉ H ₁₇ O ₇	471.093285	C ₂₃ H ₁₉ O ₁₁	525.088594	C ₂₂ H ₂₁ O ₁₅
369.134362	C ₂₁ H ₂₁ O ₆	359.040856	C ₁₇ H ₁₁ O ₉	471.129671	C ₂₄ H ₂₃ O ₁₀	525.124979	C ₂₃ H ₂₅ O ₁₄
369.170747	C ₂₂ H ₂₅ O ₅	359.077241	C ₁₈ H ₁₅ O ₈	473.072550	C ₂₂ H ₁₇ O ₁₂	527.104244	C ₂₂ H ₂₃ O ₁₅
371.150012	C ₂₁ H ₂₃ O ₆	361.071762	C ₂₁ H ₁₃ O ₆	473.108935	C ₂₃ H ₂₁ O ₁₁	533.057293	C ₂₃ H ₁₇ O ₁₅
379.155097	C ₂₃ H ₂₃ O ₅	361.108147	C ₂₂ H ₁₇ O ₅	475.088200	C ₂₂ H ₁₉ O ₁₂	533.093679	C ₂₄ H ₂₁ O ₁₄
379.191483	C ₂₄ H ₂₇ O ₄	363.051026	C ₂₀ H ₁₁ O ₇	475.124585	C ₂₃ H ₂₃ O ₁₁	533.130064	C ₂₅ H ₂₅ O ₁₃
381.134362	C ₂₂ H ₂₁ O ₆	363.087412	C ₂₁ H ₁₅ O ₆	483.129671	C ₂₅ H ₂₃ O ₁₀	533.166450	C ₂₆ H ₂₉ O ₁₂
381.170747	C ₂₃ H ₂₅ O ₅	363.123797	C ₂₂ H ₁₉ O ₅	485.108935	C ₂₄ H ₂₁ O ₁₁	535.072944	C ₂₃ H ₁₉ O ₁₅
381.207133	C ₂₄ H ₂₉ O ₄	365.030291	C ₁₉ H ₉ O ₈	485.145321	C ₂₅ H ₂₅ O ₁₀	535.109329	C ₂₄ H ₂₃ O ₁₄
383.150012	C ₂₂ H ₂₃ O ₆	365.066676	C ₂₀ H ₁₃ O ₇	487.088200	C ₂₃ H ₁₉ O ₁₂	535.145715	C ₂₅ H ₂₇ O ₁₃
383.186398	C ₂₃ H ₂₇ O ₅	365.103062	C ₂₁ H ₁₇ O ₆	487.124585	C ₂₄ H ₂₃ O ₁₁	537.052208	C ₂₂ H ₁₇ O ₁₆
385.165662	C ₂₂ H ₂₅ O ₆	367.045941	C ₁₉ H ₁₁ O ₈	489.103850	C ₂₃ H ₂₁ O ₁₂	537.088594	C ₂₃ H ₂₁ O ₁₅
393.170747	C ₂₄ H ₂₅ O ₅	367.082326	C ₂₀ H ₁₅ O ₇	499.124585	C ₂₅ H ₂₃ O ₁₁	537.124979	C ₂₄ H ₂₅ O ₁₄
395.150012	C ₂₃ H ₂₃ O ₆	367.118712	C ₂₁ H ₁₉ O ₆	501.103850	C ₂₄ H ₂₁ O ₁₂	539.067858	C ₂₂ H ₁₉ O ₁₆
395.186398	C ₂₄ H ₂₇ O ₅	369.025205	C ₁₈ H ₉ O ₉	503.119500	C ₂₄ H ₂₃ O ₁₂	539.104244	C ₂₃ H ₂₃ O ₁₅
395.222783	C ₂₅ H ₃₁ O ₄	369.061591	C ₁₉ H ₁₃ O ₈	513.140235	C ₂₆ H ₂₅ O ₁₁	547.145715	C ₂₆ H ₂₇ O ₁₃
397.165662	C ₂₃ H ₂₅ O ₆	371.040856	C ₁₈ H ₁₁ O ₉	515.119500	C ₂₅ H ₂₃ O ₁₂	551.067858	C ₂₃ H ₁₉ O ₁₆
407.150012	C ₂₄ H ₂₃ O ₆	371.077241	C ₁₉ H ₁₅ O ₈	527.119500	C ₂₆ H ₂₃ O ₁₂	551.104244	C ₂₄ H ₂₃ O ₁₅
407.222783	C ₂₆ H ₃₁ O ₄	371.113627	C ₂₀ H ₁₉ O ₇	529.135150	C ₂₆ H ₂₅ O ₁₂	553.083508	C ₂₃ H ₂₁ O ₁₆
409.165662	C ₂₄ H ₂₅ O ₆	373.071762	C ₂₂ H ₁₃ O ₆	531.114414	C ₂₅ H ₂₃ O ₁₃	553.119894	C ₂₄ H ₂₅ O ₁₅
409.202048	C ₂₅ H ₂₉ O ₅	375.051026	C ₂₁ H ₁₁ O ₇	539.155885	C ₂₈ H ₂₇ O ₁₁	553.156279	C ₂₅ H ₂₉ O ₁₄
411.144927	C ₂₃ H ₂₃ O ₇	375.087412	C ₂₂ H ₁₅ O ₆	541.171535	C ₂₈ H ₂₉ O ₁₁	565.119894	C ₂₅ H ₂₅ O ₁₅
421.165662	C ₂₅ H ₂₅ O ₆	377.066676	C ₂₁ H ₁₃ O ₇	543.150800	C ₂₇ H ₂₇ O ₁₂	565.156279	C ₂₆ H ₂₉ O ₁₄
423.217698	C ₂₆ H ₃₁ O ₅	377.103062	C ₂₂ H ₁₇ O ₆	555.150800	C ₂₈ H ₂₇ O ₁₂		
437.233348	C ₂₇ H ₃₃ O ₅	377.139447	C ₂₃ H ₂₁ O ₅	557.166450	C ₂₈ H ₂₉ O ₁₂		
439.176227	C ₂₅ H ₂₇ O ₇	379.045941	C ₂₀ H ₁₁ O ₈	569.166450	C ₂₉ H ₂₉ O ₁₂		
439.212612	C ₂₆ H ₃₁ O ₆	379.118712	C ₂₂ H ₁₉ O ₆				
453.264648	C ₂₈ H ₃₇ O ₅	381.025205	C ₁₉ H ₉ O ₉				
467.207527	C ₂₇ H ₃₁ O ₇	381.061591	C ₂₀ H ₁₃ O ₈				
467.243912	C ₂₈ H ₃₅ O ₆	381.097976	C ₂₁ H ₁₇ O ₇				

383.040856	C ₁₉ H ₁₁ O ₉
383.077241	C ₂₀ H ₁₅ O ₈
385.056506	C ₁₉ H ₁₃ O ₉
385.092891	C ₂₀ H ₁₇ O ₈
389.066676	C ₂₂ H ₁₃ O ₇
389.103062	C ₂₃ H ₁₇ O ₆
391.045941	C ₂₁ H ₁₁ O ₈
391.082326	C ₂₂ H ₁₅ O ₇
391.118712	C ₂₃ H ₁₉ O ₆
393.061591	C ₂₁ H ₁₃ O ₈
393.097976	C ₂₂ H ₁₇ O ₇
395.040856	C ₂₀ H ₁₁ O ₉
395.077241	C ₂₁ H ₁₅ O ₈
395.113627	C ₂₂ H ₁₉ O ₇
397.056506	C ₂₀ H ₁₃ O ₉
397.092891	C ₂₁ H ₁₇ O ₈
397.129277	C ₂₂ H ₂₁ O ₇
399.108541	C ₂₁ H ₁₉ O ₈
403.045941	C ₂₂ H ₁₁ O ₈
405.061591	C ₂₂ H ₁₃ O ₈
405.097976	C ₂₃ H ₁₇ O ₇
405.134362	C ₂₄ H ₂₁ O ₆
407.077241	C ₂₂ H ₁₅ O ₈
407.113627	C ₂₃ H ₁₉ O ₇
409.056506	C ₂₁ H ₁₃ O ₉
409.092891	C ₂₂ H ₁₇ O ₈
409.129277	C ₂₃ H ₂₁ O ₇
411.072156	C ₂₁ H ₁₅ O ₉
411.108541	C ₂₂ H ₁₉ O ₈
417.097976	C ₂₄ H ₁₇ O ₇
419.113627	C ₂₄ H ₁₉ O ₇
419.150012	C ₂₅ H ₂₃ O ₆
421.056506	C ₂₂ H ₁₃ O ₉
421.092891	C ₂₃ H ₁₇ O ₈
421.129277	C ₂₄ H ₂₁ O ₇
423.072156	C ₂₂ H ₁₅ O ₉
423.108541	C ₂₃ H ₁₉ O ₈
425.087806	C ₂₂ H ₁₇ O ₉
425.124191	C ₂₃ H ₂₁ O ₈
431.113627	C ₂₅ H ₁₉ O ₇
433.092891	C ₂₄ H ₁₇ O ₈
433.129277	C ₂₅ H ₂₁ O ₇
435.072156	C ₂₃ H ₁₅ O ₉
435.108541	C ₂₄ H ₁₉ O ₈
437.124191	C ₂₄ H ₂₁ O ₈
447.144927	C ₂₆ H ₂₃ O ₇
449.124191	C ₂₅ H ₂₁ O ₈

451.103456	$C_{24}H_{19}O_9$
451.139841	$C_{25}H_{23}O_8$
463.103456	$C_{25}H_{19}O_9$
463.139841	$C_{26}H_{23}O_8$
465.119106	$C_{25}H_{21}O_9$
477.119106	$C_{26}H_{21}O_9$
477.155491	$C_{27}H_{25}O_8$
479.134756	$C_{26}H_{23}O_9$
491.134756	$C_{27}H_{23}O_9$
493.150406	$C_{27}H_{25}O_9$
505.150406	$C_{28}H_{25}O_9$
507.129671	$C_{27}H_{23}O_{10}$
507.166056	$C_{28}H_{27}O_9$
525.140235	$C_{27}H_{25}O_{11}$
