Supporting Information

Refinement of compound aromaticity in complex organic mixtures by stable isotope label assisted ultra-high resolution mass spectrometry

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MATERIALS AND METHODS

Table S1. Structural group composition of BP-Cx-1 obtained by liquid-phase ^{13}C NMR spectroscopy. Values in table are relative contributions to the total integral of the particular spectrum regions.[1]

Carbon content in the structural fragments*, %						
O = CRR' (185-220 ppm)	COO (167-185 ppm)	$C_{Ar-O(H,R)}$ (145-167 ppm)	C_{Ar} (108-145 ppm)	C_{Alk-O} (90-108 ppm)	OCH_3 (48-90 ppm)	C_{Alk} (0-48 ppm)
4	6	8	45	15	7	15

* - chemical shifts for the regions are in brackets

Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

All samples were analyzed by direct-infusion negative electrospray ionization (DI ESI) on a dual-source 12T solariX XR FTICR mass spectrometer (Bruker Daltonics, Billerica, MA, U.S.A.) equipped with a dynamically harmonized cell[2,3] located at the ProVIS Centre for Chemical Microscopy within the Helmholtz Centre for Environmental Research - UFZ. Prior to analysis, samples under study were diluted with water-methanol (1:1) mixture to concentration of 50 mg/L. The mass-spectra were both externally calibrated using arginine clusters[4] and internally recalibrated calibrated by known mass peaks of fatty acids[5] reaching mass accuracy values of < 200 ppb. The spectra were acquired with a time domain of 4 megawords and 300 scans were accumulated for each spectrum. Mass resolving power was 530 000 at m/z = 400. The FTICR MS data were processed using the open source browser-based application UltraMassExplorer created by Leefmann et al. (http://dockersrv1.awi.de:3838/ume).[6] The generated CHONS formulas were validated by setting sensible chemical constraints typical for plant-derived polyphenols[7,8] (O/C ratio ≤ 1, 0.3<H/C ratio ≤ 2.2, element counts (C ≤ 120, H ≤ 200, O ≤ 60, N ≤ 2, S ≤ 1) and mass accuracy window < 0.5 ppm). The assigned CHNOS formulae were further plotted into van Krevelen and Kendrick diagrams[9].

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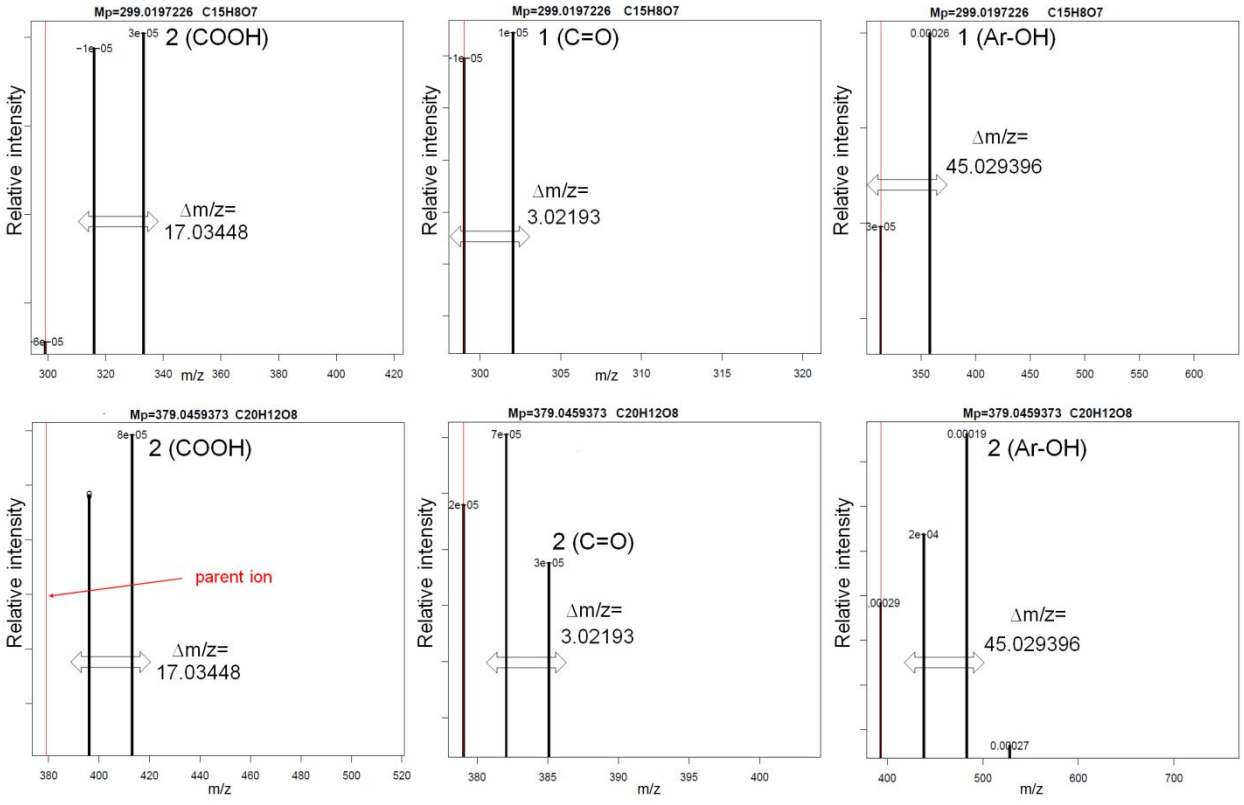

Figure S1. Examples of reconstructed mass-spectra of BP-Cx-1 samples labeled by deuteromethylation, reducing and acetylation corresponding to the enumeration of carboxylic (left panel), carbonyl (middle panel) and phenolic (right panel) groups. Red lines indicate the position of the parent ions in all cases. Formulae correspond to the neutral compounds, while masses correspond to m/z values. Errors to theoretical masses are assigned above peaks.

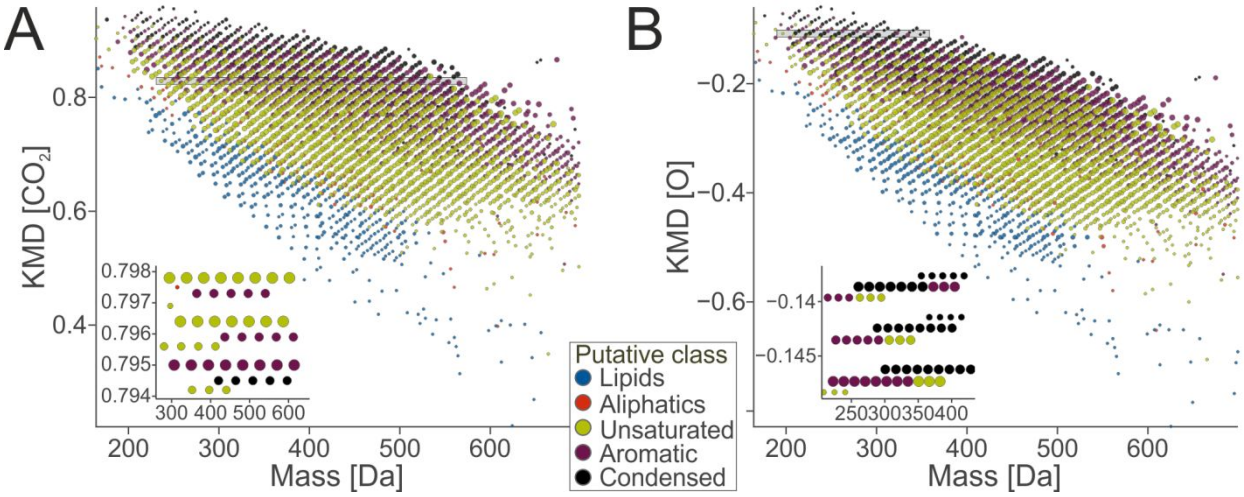

Figure S2. Molecular composition of sample BP-Cx-1. Kendrick mass defect plot for the CO_2 (A) and O (B) base mass for the 1156 CHO formulas colored by putative molecular classes. No class switch within CO_2 homologous series occurs, if molecular classes are based in AI_{mod}. For the O homologous series, molecular classes can change as highlighted in the insets. The size of the points correspond to the length of the homologous series.

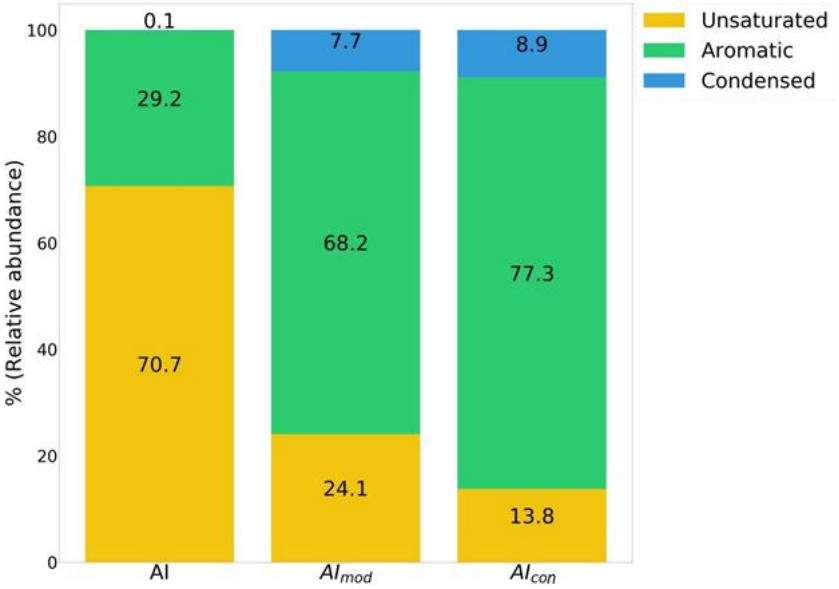

Figure S3. Relative abundance of three major classes calculated according to different aromaticity indices: AI, AI_{mod} and AI_{con}.

Table S2. Molecular components with assigned functional groups

MEASURED M/Z	MOLECULAR FORMULA	MASS ERROR [PPM]	C	H	O	COOH	C=O	R-OH	O/C	H/C	AI	AI_{MOD}	AI_{CON}
206.05791	C11H10O4	0.01047	11	10	4	2	0	1	0.36	0.91	0.43	0.56	0.56
216.04226	C12H8O4	0.00724	12	8	4	1	0	1	0.33	0.67	0.63	0.70	0.73
218.05791	C12H10O4	0.01114	12	10	4	1	2	0	0.33	0.83	0.50	0.60	0.56
220.03717	C11H8O5	0.01033	11	8	5	2	0	1	0.45	0.73	0.50	0.65	0.67
222.01644	C10H6O6	0.00957	10	6	6	2	0	0	0.60	0.60	0.50	0.71	0.75
232.07356	C13H12O4	0.01391	13	12	4	1	0	2	0.31	0.92	0.44	0.55	0.58
236.06847	C12H12O5	0.01667	12	12	5	1	0	0	0.42	1.00	0.29	0.47	0.55
240.02700	C10H8O7	0.00778	10	8	7	3	1	0	0.70	0.80	0.00	0.54	0.50
248.06847	C13H12O5	0.02295	13	12	5	2	1	1	0.38	0.92	0.38	0.52	0.50
250.01135	C11H6O7	0.00805	11	6	7	3	0	0	0.64	0.55	0.50	0.73	0.75
250.04774	C12H10O6	0.01364	12	10	6	3	0	0	0.50	0.83	0.33	0.56	0.56
254.00627	C10H6O8	0.00727	10	6	8	3	0	0	0.80	0.60	0.00	0.67	0.71
254.05791	C15H10O4	0.03	15	10	4	1	1	2	0.27	0.67	0.64	0.69	0.69
256.03717	C14H8O5	0.0203	14	8	5	1	2	2	0.36	0.57	0.67	0.74	0.73
260.03209	C13H8O6	0.01052	13	8	6	2	2	2	0.46	0.62	0.57	0.70	0.67
262.04774	C13H10O6	0.02474	13	10	6	2	1	1	0.46	0.77	0.43	0.60	0.60
262.12051	C15H18O4	0.01601	15	18	4	1	0	2	0.27	1.20	0.27	0.38	0.43
264.02700	C12H8O7	0.01125	12	8	7	2	1	0	0.58	0.67	0.40	0.65	0.67
264.06339	C13H12O6	0.01887	13	12	6	2	1	0	0.46	0.92	0.29	0.50	0.50
264.09977	C14H16O5	0.01798	14	16	5	1	0	1	0.36	1.14	0.22	0.39	0.46
266.04265	C12H10O7	0.01044	12	10	7	2	0	0	0.58	0.83	0.20	0.53	0.60
268.05830	C12H12O7	0.01261	12	12	7	3	0	0	0.58	1.00	0.00	0.41	0.44
270.05282	C15H10O5	0.06248	15	10	5	1	1	3	0.33	0.67	0.60	0.68	0.69
272.03209	C14H8O6	0.01944	14	8	6	1	1	1	0.43	0.57	0.63	0.73	0.75
272.06847	C15H12O5	0.08458	15	12	5	1	1	1	0.33	0.80	0.50	0.60	0.62
272.10486	C16H16O4	0.0189	16	16	4	1	0	2	0.25	1.00	0.42	0.50	0.53
274.04774	C14H10O6	0.02359	14	10	6	2	1	2	0.43	0.71	0.50	0.64	0.64
274.08412	C15H14O5	0.06879	15	14	5	2	0	1	0.33	0.93	0.40	0.52	0.54
278.04265	C13H10O7	0.02181	13	10	7	3	1	0	0.54	0.77	0.33	0.58	0.56
282.05282	C16H10O5	0.05713	16	10	5	1	2	0	0.31	0.63	0.64	0.70	0.69
288.02700	C14H8O7	0.01501	14	8	7	3	0	0	0.50	0.57	0.57	0.71	0.73
288.06339	C15H12O6	0.10174	15	12	6	2	1	1	0.40	0.80	0.44	0.58	0.58
288.09977	C16H16O5	0.04075	16	16	5	1	0	1	0.31	1.00	0.36	0.48	0.53
288.15729	C14H24O6	0.01569	14	24	6	1	0	0	0.43	1.71	0.00	0.00	0.15
290.04265	C14H10O7	0.02316	14	10	7	3	1	0	0.50	0.71	0.43	0.62	0.60
290.07904	C15H14O6	0.06685	15	14	6	1	0	1	0.40	0.93	0.33	0.50	0.57
292.05830	C14H12O7	0.02083	14	12	7	3	1	0	0.50	0.86	0.29	0.52	0.50
292.09469	C15H16O6	0.04504	15	16	6	2	1	1	0.40	1.07	0.22	0.42	0.42
296.03209	C16H8O6	0.01709	16	8	6	1	2	0	0.38	0.50	0.70	0.77	0.77
296.05322	C13H12O8	0.01179	13	12	8	3	0	0	0.62	0.92	0.00	0.44	0.50
296.06847	C17H12O5	0.05978	17	12	5	1	1	2	0.29	0.71	0.58	0.66	0.67
298.04774	C16H10O6	0.06781	16	10	6	2	2	2	0.38	0.63	0.60	0.69	0.67
298.08412	C17H14O5	0.0748	17	14	5	1	1	2	0.29	0.82	0.50	0.59	0.60

300.02700	C15H8O7	0.02083	15	8	7	2	1	1	0.47	0.53	0.63	0.74	0.75
302.04265	C15H10O7	0.02334	15	10	7	1	1	1	0.47	0.67	0.50	0.65	0.69
302.07904	C16H14O6	0.17342	16	14	6	0	2	0	0.38	0.88	0.40	0.54	0.57
302.11542	C17H18O5	0.02095	17	18	5	1	0	0	0.29	1.06	0.33	0.45	0.50
304.05830	C15H12O7	0.05056	15	12	7	2	1	2	0.47	0.80	0.38	0.57	0.58
304.09469	C16H16O6	0.05592	16	16	6	1	0	1	0.38	1.00	0.30	0.46	0.53
306.11034	C16H18O6	0.04168	16	18	6	2	0	1	0.38	1.13	0.20	0.38	0.43
308.05322	C14H12O8	0.01483	14	12	8	1	0	0	0.57	0.86	0.17	0.50	0.62
308.08960	C15H16O7	0.01939	15	16	7	2	0	0	0.47	1.07	0.13	0.39	0.46
308.12599	C16H20O6	0.02358	16	20	6	2	0	1	0.38	1.25	0.10	0.31	0.36
310.04774	C17H10O6	0.02293	17	10	6	1	2	0	0.35	0.59	0.64	0.71	0.71
310.08412	C18H14O5	0.02977	18	14	5	1	1	1	0.28	0.78	0.54	0.61	0.63
312.02700	C16H8O7	0.01016	16	8	7	2	1	2	0.44	0.50	0.67	0.76	0.77
312.06339	C17H12O6	0.03117	17	12	6	2	2	1	0.35	0.71	0.55	0.64	0.62
312.09977	C18H16O5	0.02259	18	16	5	0	1	2	0.28	0.89	0.46	0.55	0.59
314.04265	C16H10O7	0.09069	16	10	7	2	1	2	0.44	0.63	0.56	0.68	0.69
314.11542	C18H18O5	0.03955	18	18	5	1	1	2	0.28	1.00	0.38	0.48	0.50
316.02192	C15H8O8	0.01329	15	8	8	3	1	0	0.53	0.53	0.57	0.73	0.73
316.05830	C16H12O7	0.1124	16	12	7	2	1	1	0.44	0.75	0.44	0.60	0.62
316.09469	C17H16O6	0.11434	17	16	6	2	1	1	0.35	0.94	0.36	0.50	0.50
318.07395	C16H14O7	0.25122	16	14	7	2	1	0	0.44	0.88	0.33	0.52	0.54
320.05322	C15H12O8	0.01962	15	12	8	2	1	0	0.53	0.80	0.29	0.55	0.58
320.08960	C16H16O7	0.03712	16	16	7	3	0	1	0.44	1.00	0.22	0.44	0.46
322.06887	C15H14O8	0.02095	15	14	8	3	0	0	0.53	0.93	0.14	0.45	0.50
322.10525	C16H18O7	0.02204	16	18	7	2	0	0	0.44	1.13	0.11	0.36	0.43
322.14164	C17H22O6	0.01884	17	22	6	1	0	1	0.35	1.29	0.09	0.29	0.38
324.06339	C18H12O6	0.03456	18	12	6	1	2	0	0.33	0.67	0.58	0.67	0.67
326.07904	C18H14O6	0.03685	18	14	6	1	2	0	0.33	0.78	0.50	0.60	0.60
328.02192	C16H8O8	0.02531	16	8	8	3	1	2	0.50	0.50	0.63	0.75	0.75
328.05830	C17H12O7	0.06793	17	12	7	2	2	2	0.41	0.71	0.50	0.63	0.62
328.09469	C18H16O6	0.16799	18	16	6	1	1	1	0.33	0.89	0.42	0.53	0.56
330.03757	C16H10O8	0.06502	16	10	8	2	1	0	0.50	0.63	0.50	0.67	0.69
330.07395	C17H14O7	0.11175	17	14	7	2	2	1	0.41	0.82	0.40	0.56	0.54
330.11034	C18H18O6	0.1128	18	18	6	1	1	1	0.33	1.00	0.33	0.47	0.50
332.05322	C16H12O8	0.06833	16	12	8	3	1	1	0.50	0.75	0.38	0.58	0.58
332.08960	C17H16O7	0.15964	17	16	7	2	1	0	0.41	0.94	0.30	0.48	0.50
332.12599	C18H20O6	0.05055	18	20	6	0	0	0	0.33	1.11	0.25	0.40	0.50
334.06887	C16H14O8	0.13918	16	14	8	2	0	0	0.50	0.88	0.25	0.50	0.57
336.04813	C15H12O9	0.01361	15	12	9	3	0	0	0.60	0.80	0.17	0.52	0.58
336.08452	C16H16O8	0.02609	16	16	8	3	1	0	0.50	1.00	0.13	0.42	0.42
338.07904	C19H14O6	0.0407	19	14	6	1	1	2	0.32	0.74	0.54	0.63	0.65
338.10017	C16H18O8	0.01021	16	18	8	2	0	0	0.50	1.13	0.00	0.33	0.43
340.02192	C17H8O8	0.01042	17	8	8	2	2	1	0.47	0.47	0.67	0.77	0.77
340.05830	C18H12O7	0.02356	18	12	7	2	2	2	0.39	0.67	0.55	0.66	0.64
340.09469	C19H16O6	0.0347	19	16	6	1	1	2	0.32	0.84	0.46	0.56	0.59
342.03757	C17H10O8	0.05176	17	10	8	3	2	1	0.47	0.59	0.56	0.69	0.67
342.07395	C18H14O7	0.11575	18	14	7	2	1	1	0.39	0.78	0.45	0.59	0.60
342.11034	C19H18O6	0.06302	19	18	6	1	1	0	0.32	0.95	0.38	0.50	0.53
344.01683	C16H8O9	0.01513	16	8	9	2	1	0	0.56	0.50	0.57	0.74	0.77

344.08960	C18H16O7	0.15153	18	16	7	3	2	0	0.39	0.89	0.36	0.52	0.46
344.12599	C19H20O6	0.06938	19	20	6	1	1	0	0.32	1.05	0.31	0.44	0.47
346.03248	C16H10O9	0.0221	16	10	9	3	2	0	0.56	0.63	0.43	0.65	0.64
346.06887	C17H14O8	0.26043	17	14	8	3	2	1	0.47	0.82	0.33	0.54	0.50
346.10525	C18H18O7	0.17437	18	18	7	3	2	0	0.39	1.00	0.27	0.45	0.38
348.08452	C17H16O8	0.05385	17	16	8	3	0	0	0.47	0.94	0.22	0.46	0.50
348.12090	C18H20O7	0.0787	18	20	7	2	0	0	0.39	1.11	0.18	0.38	0.44
350.07904	C20H14O6	0.13016	20	14	6	1	1	2	0.30	0.70	0.57	0.65	0.67
350.10017	C17H18O8	0.03464	17	18	8	3	0	0	0.47	1.06	0.11	0.38	0.43
352.11582	C17H20O8	0.02081	17	20	8	3	0	0	0.47	1.18	0.00	0.31	0.36
354.03757	C18H10O8	0.03178	18	10	8	2	2	0	0.44	0.56	0.60	0.71	0.71
354.07395	C19H14O7	0.1056	19	14	7	2	2	1	0.37	0.74	0.50	0.61	0.60
354.11034	C20H18O6	0.07811	20	18	6	1	1	0	0.30	0.90	0.43	0.53	0.56
356.01683	C17H8O9	0.01423	17	8	9	2	2	0	0.53	0.47	0.63	0.76	0.77
356.05322	C18H12O8	0.05503	18	12	8	3	1	1	0.44	0.67	0.50	0.64	0.64
356.08960	C19H16O7	0.13557	19	16	7	2	1	0	0.37	0.84	0.42	0.55	0.56
356.12599	C20H20O6	0.05883	20	20	6	0	1	2	0.30	1.00	0.36	0.47	0.53
358.03248	C17H10O9	0.02046	17	10	9	2	1	0	0.53	0.59	0.50	0.68	0.71
360.08452	C18H16O8	0.0932	18	16	8	2	0	0	0.44	0.89	0.30	0.50	0.56
362.06378	C17H14O9	0.04395	17	14	9	3	1	0	0.53	0.82	0.25	0.52	0.54
362.10017	C18H18O8	0.0718	18	18	8	2	0	0	0.44	1.00	0.20	0.43	0.50
362.13655	C19H22O7	0.04397	19	22	7	1	0	0	0.37	1.16	0.17	0.35	0.44
364.05830	C20H12O7	0.04664	20	12	7	2	1	2	0.35	0.60	0.62	0.70	0.71
364.09469	C21H16O6	0.10725	21	16	6	1	1	2	0.29	0.76	0.53	0.61	0.63
366.03757	C19H10O8	0.01899	19	10	8	2	1	1	0.42	0.53	0.64	0.73	0.75
366.07395	C20H14O7	0.11416	20	14	7	2	1	1	0.35	0.70	0.54	0.64	0.65
366.09508	C17H18O9	0.02124	17	18	9	3	0	0	0.53	1.06	0.00	0.36	0.43
368.01683	C18H8O9	0.01959	18	8	9	3	1	1	0.50	0.44	0.67	0.78	0.79
368.08960	C20H16O7	0.11829	20	16	7	2	2	2	0.35	0.80	0.46	0.58	0.56
372.04813	C18H12O9	0.0737	18	12	9	4	2	1	0.50	0.67	0.44	0.63	0.58
372.12090	C20H20O7	0.19105	20	20	7	1	2	0	0.35	1.00	0.31	0.45	0.47
374.06378	C18H14O9	0.04994	18	14	9	2	2	0	0.50	0.78	0.33	0.56	0.57
374.13655	C20H22O7	0.08752	20	22	7	1	0	0	0.35	1.10	0.23	0.39	0.47
376.07943	C18H16O9	0.04017	18	16	9	3	2	0	0.50	0.89	0.22	0.48	0.46
376.11582	C19H20O8	0.08179	19	20	8	2	0	0	0.42	1.05	0.18	0.40	0.47
376.15220	C20H24O7	0.03861	20	24	7	1	0	1	0.35	1.20	0.15	0.33	0.42
378.07395	C21H14O7	0.09371	21	14	7	2	1	2	0.33	0.67	0.57	0.66	0.67
380.05322	C20H12O8	0.03485	20	12	8	2	2	2	0.40	0.60	0.58	0.69	0.69
380.08960	C21H16O7	0.10331	21	16	7	2	1	1	0.33	0.76	0.50	0.60	0.61
382.06887	C20H14O8	0.06841	20	14	8	3	1	2	0.40	0.70	0.50	0.63	0.63
384.04813	C19H12O9	0.05103	19	12	9	3	1	1	0.47	0.63	0.50	0.66	0.67
384.08452	C20H16O8	0.15179	20	16	8	2	2	0	0.40	0.80	0.42	0.56	0.56
386.02740	C18H10O10	0.0374	18	10	10	3	1	0	0.56	0.56	0.50	0.69	0.71
386.06378	C19H14O9	0.07913	19	14	9	3	2	0	0.47	0.74	0.40	0.59	0.57
386.10017	C20H18O8	0.14912	20	18	8	2	1	0	0.40	0.90	0.33	0.50	0.53
386.13655	C21H22O7	0.17335	21	22	7	1	1	0	0.33	1.05	0.29	0.43	0.47
388.07943	C19H16O9	0.08753	19	16	9	3	1	0	0.47	0.84	0.30	0.52	0.53
390.05870	C18H14O10	0.03263	18	14	10	3	0	0	0.56	0.78	0.25	0.54	0.60
392.08960	C22H16O7	0.13537	22	16	7	1	1	3	0.32	0.73	0.53	0.62	0.65

392.11073	C19H20O9	0.04106	19	20	9	2	0	0	0.47	1.05	0.10	0.38	0.47
396.04813	C20H12O9	0.03298	20	12	9	2	3	0	0.45	0.60	0.55	0.68	0.67
396.08452	C21H16O8	0.1066	21	16	8	3	1	2	0.38	0.76	0.46	0.59	0.59
396.12090	C22H20O7	0.1139	22	20	7	2	1	0	0.32	0.91	0.40	0.51	0.53
398.06378	C20H14O9	0.06804	20	14	9	3	3	1	0.45	0.70	0.45	0.61	0.57
398.10017	C21H18O8	0.11664	21	18	8	3	1	1	0.38	0.86	0.38	0.53	0.53
400.04305	C19H12O10	0.0378	19	12	10	3	1	1	0.53	0.63	0.44	0.64	0.67
400.07943	C20H16O9	0.08648	20	16	9	3	1	0	0.45	0.80	0.36	0.55	0.56
400.11582	C21H20O8	0.14555	21	20	8	2	1	0	0.38	0.95	0.31	0.47	0.50
402.07395	C23H14O7	0.06806	23	14	7	1	1	2	0.30	0.61	0.63	0.69	0.71
402.09508	C20H18O9	0.09077	20	18	9	3	1	0	0.45	0.90	0.27	0.48	0.50
404.07435	C19H16O10	0.03204	19	16	10	3	1	0	0.53	0.84	0.22	0.50	0.53
404.11073	C20H20O9	0.08616	20	20	9	3	0	0	0.45	1.00	0.18	0.42	0.47
406.06887	C22H14O8	0.08895	22	14	8	2	1	2	0.36	0.64	0.57	0.67	0.68
408.04813	C21H12O9	0.04371	21	12	9	3	2	2	0.43	0.57	0.58	0.70	0.69
408.08452	C22H16O8	0.13305	22	16	8	2	2	1	0.36	0.73	0.50	0.61	0.61
408.17842	C21H28O8	0.01467	21	28	8	0	0	1	0.38	1.33	0.00	0.24	0.38
410.10017	C22H18O8	0.16512	22	18	8	2	1	2	0.36	0.82	0.43	0.56	0.58
410.13655	C23H22O7	0.08409	23	22	7	1	1	0	0.30	0.96	0.38	0.49	0.52
412.07943	C21H16O9	0.08835	21	16	9	3	1	0	0.43	0.76	0.42	0.58	0.59
412.11582	C22H20O8	0.14933	22	20	8	2	2	1	0.36	0.91	0.36	0.50	0.50
414.13147	C22H22O8	0.12224	22	22	8	2	1	1	0.36	1.00	0.29	0.44	0.47
416.08960	C24H16O7	0.07462	24	16	7	1	1	2	0.29	0.67	0.59	0.66	0.68
416.11073	C21H20O9	0.11708	21	20	9	2	1	0	0.43	0.95	0.25	0.45	0.50
418.12638	C21H22O9	0.11321	21	22	9	2	1	0	0.43	1.05	0.17	0.39	0.44
420.04813	C22H12O9	0.0351	22	12	9	2	1	1	0.41	0.55	0.62	0.71	0.74
420.08452	C23H16O8	0.1199	23	16	8	2	1	2	0.35	0.70	0.53	0.63	0.65
420.12090	C24H20O7	0.13498	24	20	7	0	1	1	0.29	0.83	0.47	0.56	0.61
422.06378	C22H14O9	0.06129	22	14	9	3	1	1	0.41	0.64	0.54	0.66	0.67
422.10017	C23H18O8	0.16064	23	18	8	2	2	1	0.35	0.78	0.47	0.58	0.58
424.07943	C22H16O9	0.07887	22	16	9	3	1	2	0.41	0.73	0.46	0.60	0.61
424.11582	C23H20O8	0.17392	23	20	8	1	2	2	0.35	0.87	0.40	0.53	0.55
428.07435	C21H16O10	0.05859	21	16	10	3	1	0	0.48	0.76	0.36	0.56	0.59
430.09000	C21H18O10	0.0606	21	18	10	3	0	0	0.48	0.86	0.27	0.50	0.56
434.10017	C24H18O8	0.15062	24	18	8	2	3	2	0.33	0.75	0.50	0.60	0.58
436.04305	C22H12O10	0.02885	22	12	10	3	1	1	0.45	0.55	0.58	0.71	0.72
436.11582	C24H20O8	0.14712	24	20	8	2	2	1	0.33	0.83	0.44	0.55	0.55
438.13147	C24H22O8	0.14836	24	22	8	1	1	1	0.33	0.92	0.38	0.50	0.55
440.07435	C22H16O10	0.05579	22	16	10	4	1	0	0.45	0.73	0.42	0.59	0.59
442.09000	C22H18O10	0.05799	22	18	10	3	1	0	0.45	0.82	0.33	0.53	0.56
446.06378	C24H14O9	0.05263	24	14	9	3	2	2	0.38	0.58	0.60	0.69	0.68
446.10017	C25H18O8	0.15913	25	18	8	2	1	1	0.32	0.72	0.53	0.62	0.64
448.07943	C24H16O9	0.10185	24	16	9	2	3	1	0.38	0.67	0.53	0.64	0.63
448.11582	C25H20O8	0.12955	25	20	8	1	1	2	0.32	0.80	0.47	0.57	0.61
450.16785	C26H26O7	0.04757	26	26	7	0	0	0	0.27	1.00	0.37	0.47	0.54
452.07435	C23H16O10	0.07288	23	16	10	3	1	1	0.43	0.70	0.46	0.61	0.63
452.11073	C24H20O9	0.14687	24	20	9	2	1	0	0.38	0.83	0.40	0.54	0.57
454.05361	C22H14O11	0.02624	22	14	11	3	1	0	0.50	0.64	0.45	0.64	0.67
454.09000	C23H18O10	0.08931	23	18	10	3	2	0	0.43	0.78	0.38	0.56	0.56

456.10565	C23H20O10	0.07229	23	20	10	3	1	1	0.43	0.87	0.31	0.50	0.53
456.14203	C24H24O9	0.09412	24	24	9	2	1	0	0.38	1.00	0.27	0.44	0.48
460.11582	C26H20O8	0.09064	26	20	8	1	1	1	0.31	0.77	0.50	0.59	0.63
462.05870	C24H14O10	0.04629	24	14	10	3	3	1	0.42	0.58	0.57	0.68	0.67
462.09508	C25H18O9	0.11051	25	18	9	1	2	1	0.36	0.72	0.50	0.61	0.64
462.13147	C26H22O8	0.13388	26	22	8	1	1	2	0.31	0.85	0.44	0.55	0.58
464.07435	C24H16O10	0.06819	24	16	10	3	2	2	0.42	0.67	0.50	0.63	0.63
470.12130	C24H22O10	0.094	24	22	10	3	1	1	0.42	0.92	0.29	0.47	0.50
472.11582	C27H20O8	0.09696	27	20	8	1	1	2	0.30	0.74	0.53	0.61	0.64
476.07435	C25H16O10	0.04144	25	16	10	3	1	1	0.40	0.64	0.53	0.65	0.67
476.11073	C26H20O9	0.07834	26	20	9	2	2	2	0.35	0.77	0.47	0.58	0.59
478.09000	C25H18O10	0.07124	25	18	10	3	3	1	0.40	0.72	0.47	0.60	0.58
480.06926	C24H16O11	0.05614	24	16	11	3	1	0	0.46	0.67	0.46	0.62	0.65
480.10565	C25H20O10	0.10142	25	20	10	3	1	1	0.40	0.80	0.40	0.55	0.57
480.14203	C26H24O9	0.15438	26	24	9	2	1	0	0.35	0.92	0.35	0.49	0.52
486.09508	C27H18O9	0.08036	27	18	9	1	1	2	0.33	0.67	0.56	0.64	0.68
488.07435	C26H16O10	0.04077	26	16	10	2	2	2	0.38	0.62	0.56	0.67	0.68
490.09000	C26H18O10	0.06398	26	18	10	2	2	1	0.38	0.69	0.50	0.62	0.64
490.12638	C27H22O9	0.12366	27	22	9	2	1	1	0.33	0.81	0.44	0.56	0.58
492.06926	C25H16O11	0.04817	25	16	11	3	1	1	0.44	0.64	0.50	0.64	0.67
492.10565	C26H20O10	0.11928	26	20	10	2	1	1	0.38	0.77	0.44	0.57	0.61
494.15768	C27H26O9	0.14004	27	26	9	1	1	0	0.33	0.96	0.33	0.47	0.52
498.11621	C25H22O11	0.05218	25	22	11	3	1	0	0.44	0.88	0.29	0.49	0.52