Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Analysis of high-molecular-weight fructan polymers in crude plant extracts by high-resolution LC-MS

Scott Harrison

Table S1 Monoisotopic masses of fructan polymers between DP1 and 108, showing formula, elemental composition and expected m/z for charge states -1 and -6. The normally observed charge states are highlighted

			ental Compo		Cl		no-Isotpic Mass			let -
	Molecular Formula	С	H	0	Charge -1	Charge -2	Charge -3	Charge -4	Charge -5	Charge -6
	1 C6H12O6 2 C12H22O11	12		6 11	179.055620 341.108495	89.023895 170.050333	59.013320 113.030945	44.008033 84.521251	35.004860 67.415435	29.0027 56.0115
	3 C18H32O16	18	_	16	503.161370	251.076770	167.048570	125.034470	99.826010	83.0203
	4 C24H42O21	24	42	21	665.214245	332.103208	221.066195	165.547689	132.236585	110.0291
	C30H52O26	30		26	827.267120	413.129645	275.083820	206.060908	164.647160	137.0379
	6 C36H62O31 7 C42H72O36	36 42	62 72	31 36	989.319995 1151.372870	494.156083 575.182520	329.101445 383.119070	246.574126 287.087345	197.057735 229.468310	164.0468 191.0556
	8 C48H82O41	48		41	1313.425745	656.208958	437.136695	327.600564	261.878885	218.0644
	9 C54H92O46	54		46	1475.478620	737.235395	491.154320	368.113783	294.289460	245.0732
	C60H102O51	60		51	1637.531495	818.261833	545.171945	408.627001	326.700035	272.0820
	1 C66H112O56 2 C72H122O61	72		56 61	1799.584370 1961.637245	899.288270 980.314708	599.189570 653.207195	449.140220 489.653439	359.110610 391.521185	299.0908 326.0996
	3 C78H132O66	78		66	2123.690120	1061.341145	707.224820	530.166658	423.931760	353.1084
	4 C84H142O71	84	142	71	2285.742995	1142.367583	761.242445	570.679876	456.342335	380.1173
	5 C90H152O76	90		76	2447.795870	1223.394020	815.260070	611.193095	488.752910	407.1261
	6 C96H162O81 7 C102H172O86	96	162 172	81 86	2609.848745 2771.901620	1304.420458 1385.446895	869.277695	651.706314	521.163485 553.574060	434.1349
	8 C108H182O91	102		91	2933.954495	1466.473333	923.295320 977.312945	692.219533 732.732751	585.984635	461.1437 488.1525
	9 C114H192O96	114		96	3096.007370	1547.499770	1031.330570	773.245970	618.395210	515.1613
	C120H202O101	120		101	3258.060245	1628.526208	1085.348195	813.759189	650.805785	542.1701
	1 C126H212O106	126	212	106 111	3420.113120	1709.552645	1139.365820	854.272408	683.216360	569.1789
	2 C132H222O111 3 C138H232O116	132	_	111	3582.165995 3744.218870	1790.579083 1871.605520	1193.383445 1247.401070	894.785626 935.298845	715.626935 748.037510	596.1878 623.1966
	4 C144H242O121	144	242	121	3906.271745	1952.631958	1301.418695	975.812064	780.448085	650.2054
2.	5 C150H252O126	150	252	126	4068.324620	2033.658395	1355.436320	1016.325283	812.858660	677.2142
	6 C156H262O131	156		131	4230.377495	2114.684833	1409.453945	1056.838501	845.269235	704.2230
	7 C162H272O136 8 C168H282O141	162 168	272	136 141	4392.430370 4554.483245	2195.711270 2276.737708	1463.471570 1517.489195	1097.351720 1137.864939	910.090385	731.2318 758.2406
	9 C174H292O146	174		141	4716.536120	2357.764145	1571.506820	1178.378158	942.500960	785.2494
	C180H302O151	180		151	4878.588995	2438.790583	1625.524445	1218.891376	974.911535	812.2583
	1 C186H312O156	186		156	5040.641870	2519.817020	1679.542070	1259.404595	1007.322110	839.2671
	2 C192H322O161	192	322	161	5202.694745	2600.843458	1733.559695	1299.917814	1039.732685	866.2759
	3 C198H332O166 4 C204H342O171	198		166 171	5364.747620 5526.800495	2681.869895 2762.896333	1787.577320 1841.594945	1340.431033 1380.944251	1072.143260 1104.553835	893.2847 920.2935
	5 C210H352O176	210		176	5688.853370	2843.922770	1895.612570	1421.457470		947.3023
3	6 C216H362O181	216	362	181	5850.906245	2924.949208	1949.630195	1461.970689	1169.374985	974.3111
	7 C222H372O186	222	372	186	6012.959120	3005.975645	2003.647820	1502.483908	1201.785560	1001.3199
	8 C228H382O191	228	382 392	191 196	6175.011995	3087.002083	2057.665445 2111.683070	1542.997126	1234.196135	1028.3288
	9 C234H392O196 0 C240H402O201	234		201	6337.064870 6499.117745	3168.028520 3249.054958	2111.683070	1583.510345 1624.023564	1266.606710 1299.017285	1055.3376
	1 C246H412O206	246		206	6661.170620	3330.081395	2219.718320	1664.536783	1331.427860	
4.	2 C252H422O211	252	422	211	6823.223495	3411.107833	2273.735945	1705.050001	1363.838435	1136.3640
	3 C258H432O216	258		216	6985.276370	3492.134270	2327.753570		1396.249010	
	4 C264H442O221 5 C270H452O226	264 270		221 226	7147.329245 7309.382120	3573.160708 3654.187145	2381.771195 2435.788820	1786.076439 1826.589658	1428.659585 1461.070160	1190.3816
	6 C276H462O231	276		231	7471.434995	3735.213583	2489.806445	1867.102876	1493.480735	1244.3993
	7 C282H472O236	282	472	236	7633.487870	3816.240020	2543.824070		1525.891310	
	8 C288H482O241	288		241	7795.540745	3897.266458	2597.841695	1948.129314	1558.301885	1298.4169
4		294		246	7957.593620	3978.292895	2651.859320		1590.712460	
	C300H502O251 1 C306H512O256	300	_	251 256	8119.646495 8281.699370	4059.319333 4140.345770	2705.876945 2759.894570	2029.155751 2069.668970	1623.123035 1655.533610	1352.4345
	2 C312H522O261	312	522	261	8443.752245	4221.372208	2813.912195	2110.182189	1687.944185	1406.4521
5	3 C318H532O266	318		266	8605.805120	4302.398645	2867.929820	2150.695408	1720.354760	1433.4609
	4 C324H542O271	324		271	8767.857995	4383.425083	2921.947445	2191.208626	1752.765335	1460.4698
	5 C330H552O276 6 C336H562O281	330		276 281	8929.910870	4464.451520	2975.965070	2231.721845 2272.235064	1785.175910	
5	+	336	562 572	281	9091.963745 9254.016620	4545.477958 4626.504395	3029.982695 3084.000320		1817.586485 1849.997060	1514.4874 1541.4962
	8 C348H582O291	348		291	9416.069495	4707.530833	3138.017945	2353.261501	1882.407635	1568.5050
	9 C354H592O296	354	592	296	9578.122370	4788.557270	3192.035570	2393.774720	1914.818210	1595.5138
	C360H602O301	360		301				2434.287939		
	1 C366H612O306 2 C372H622O311	366 372	612 622	306 311	9902.228120 10064.280995	4950.610145 5031.636583	3300.070820 3354.088445	2474.801158 2515.314376		1676.5403
	3 C378H632O316	378			10226.333870	5112.663020	3408.106070		2044.460510	
	4 C384H642O321	384			10388.386745	5193.689458	3462.123695			
	C390H652O326	390			10550.439620	5274.715895	3516.141320		2109.281660	
	6 C396H662O331	396			10712.492495	5355.742333	3570.158945		2141.692235	
	7 C402H672O336 8 C408H682O341	402	672 682	336	10874.545370 11036.598245	5436.768770 5517.795208	3624.176570 3678.194195	2717.880470 2758.393689	2174.102810 2206.513385	1811.5843 1838.5933
	9 C414H692O346	414			11198.651120	5598.821645	3732.211820			
7	C420H702O351	420	702	351	11360.703995	5679.848083	3786.229445	2839.420126		1892.6108
	1 C426H712O356	426			11522.756870	5760.874520	3840.247070			
	2 C432H722O361	432	722		11684.809745	5841.900958	3894.264695		2336.155685	1946.6284
	3 C438H732O366 4 C444H742O371	438		366	11846.862620 12008.915495	5922.927395 6003.953833	3948.282320 4002.299945	2960.959783 3001.473001	2368.566260 2400.976835	1973.6372
	5 C450H752O376	450			12170.968370	6084.980270	4056.317570			
	6 C456H762O381	456		381		6166.006708	4110.335195	3082.499439	2465.797985	2054.6636
	7 C462H772O386	462			12495.074120	6247.033145	4164.352820			
	8 C468H782O391 9 C474H792O396	468 474			12657.126995 12819.179870	6328.059583 6409.086020	4218.370445 4272.388070			2108.6813
	0 C480H802O401	480			12981.232745	6490.112458	4326.405695	3244.552314		2162.6989
8	1 C486H812O406	486	812	406	13143.285620	6571.138895	4380.423320	3285.065533	2627.850860	2189.707
	2 C492H822O411	492			13305.338495	6652.165333	4434.440945	3325.578751	2660.261435	2216.7165
	3 C498H832O416	498			13467.391370	6733.191770		3366.091970		
	4 C504H842O421 5 C510H852O426	504 510	842 852	421 426	13629.444245 13791.497120	6814.218208 6895.244645	4542.476195 4596.493820	3406.605189 3447.118408		2270.734
	6 C516H862O431	516			13953.549995	6976.271083	4650.511445	3487.631626		2324.751
8	7 C522H872O436	522	872	436	14115.602870	7057.297520	4704.529070	3528.144845	2822.314310	2351.760
	8 C528H882O441	528		441		7138.323958	4758.546695	3568.658064		2378.769
	9 C534H892O446 0 C540H902O451	534 540		446 451	14439.708620 14601.761495	7219.350395 7300.376833	4812.564320 4866.581945	3609.171283 3649.684501	2887.135460 2919.546035	2405.778
	1 C546H912O456	546			14763.814370	7300.376833	4920.599570			
	2 C552H922O461	552	922		14925.867245	7462.429708	4974.617195	3730.710939		2486.8046
9:	3 C558H932O466	558		466	15087.920120	7543.456145	5028.634820	3771.224158	3016.777760	2513.8134
	4 C564H942O471	564		471		7624.482583	5082.652445			2540.822
	5 C570H952O476 6 C576H962O481	570 576		476 481	15412.025870 15574.078745	7705.509020 7786.535458	5136.670070 5190.687695	3852.250595 3892.763814		2567.831 2594.839
	7 C582H972O486	576	962	_	15736.131620	7/86.535458 7867.561895	5190.687695			
_	8 C588H982O491	588		491		7948.588333	5298.722945		3178.830635	2648.857
9	9 C594H992O496	594	992	496	16060.237370	8029.614770	5352.740570	4014.303470	3211.241210	2675.866
	0 C600H1002O501	600			16222.290245	8110.641208	5406.758195	4054.816689		2702.875
	1 C606H1012O506	606		506 511		8191.667645	5460.775820			2729.8839
	2 C612H1022O511 3 C618H1032O516	612	1022	511 516	16546.395995 16708.448870	8272.694083 8353.720520	5514.793445 5568.811070	4135.843126 4176.356345	3308.472935 3340.883510	2756.8928
	4 C624H1042O521	624		521		8434.746958	5622.828695	4216.869564		2810.9104
10	5 C630H1052O526	630	1052	526	17032.554620	8515.773395	5676.846320	4257.382783	3405.704660	2837.9192
	6 C636H1062O531	636		531		8596.799833	5730.863945	4297.896001	3438.115235	2864.9280
10	7 C642H1072O536	642	1072	536	17356.660370	8677.826270	5784.881570	4338.409220	3470.525810	2891.936

Table S2 Monoisotopic, singly negatively charged mass, expected m/z value and relative intensity as calculated by IDCalc, for DP1,10, 20, 30, 40, 50, 60, 70, 80 and 90 at the observed charge state. Most intense isotopic peak highlighted in yellow

										200 (0.00)									
DP&Charge State		ļ								Ions (Ab	ove1%)								
DP1 -1	Isotopic Mass (da)	180.063	181.066	182.068															
	Singly Charged Ionic Mass	179.056	180.059	181.061															
	Expected m/z	179.056	180.059	181.061															
	Rel. Abu.	100.000	6.974	1.437															
DP10 -	Isotopic Mass (da)	1638.539	1639.541	1640.544	1641.546	1642.548	1643.551												
	Singly Charged Ionic Mass	1637.532	1638.534	1639.536	1640.539	1641.541	1642.543												
	Expected m/z	1637.532	1638.534	1639.536	1640.539	1641.541	1642.543												
	Rel. Abu.	100.000	69.139	33.995	12.486	3.862	1.032												
DP20 -	2 Isotopic Mass (da)	3259.067	3260.069	3261.072	3262.074	3263.076	3264.079	3265.081	3266.083										
	Singly Charged Ionic Mass	3258.060	3259.062	3260.065	3261.067	3262.069	3263.072	3264.074	3265.076										
	Expected m/z	1629.030	1629.531	1630.032	1630.533	1631.035	1631.536	1632.037	1632.538										
	Rel. Abu.	72.353	100.000	83.564	51.818	26.237	11.376	4.356	1.503										
DP30 -3	Isotopic Mass (da)	4879.595	4880.598	4881.600	4882.602	4883.605	4884.607	4885.609	4886.612	4887.614	4888.617								
	Singly Charged Ionic Mass	4878.588	4879.591	4880.593	4881.595	4882.598	4883.600	4884.602	4885.605	4886.607	4887.609								
	Expected m/z	1626.196	1626.530	1626.864	1627.198	1627.533	1627.867	1628.201	1628.535	1628.869	1629.203								
	Rel. Abu.	40.866	84.708	100.000	85.962	59.467	34.901	17.956	8.279	3.476	1.345								
	2000 N 600 C 200 C 400 V 100 C				630003000		20.23.810.	3.57.0.53.0.5		50.00.00									
DP40 -4	Isotopic Mass (da)	6500.124	6501.126	6502.128	6503.131	6504.133	6505.135	6506.138	6507.140	6508.142	6509.145	6510.147	6511.149						
	Singly Charged Ionic Mass	6499.116	6500,119	6501.121	6502.123	6503,126	6504.128	6505.130	6506,133	6507.135	6508.137	6509,140	6510.142						-
	Expected m/z	1624.779	1625,030	1625,280	1625.531	1625.781	1626.032	1626.283	1626,533	1626.784	1627.034	1627.285	1627.536						
	Rel. Abu.	21.662	59.863	91.331	100.000	87,235	64.097	41.056	23,464	12.167	5.797	2.562	1.059				1		-
	101.7104.	21.002	33.003	71.551	100.000	07.233	01.057	11.050	25.101	12.107	5.777	2.502	1.057						
DP50 -4	Isotopic Mass (da)	8120.652	8121.654	8122.656	8123.659	8124.661	8125.664	8126.666	8127.668	8128.671	8129.673	8130.675	8131.678	8132.680	8133.682				
DI 30 -4	Singly Charged Ionic Mass	8119.645	8120.647	8121.649	8122.652	8123.654	8124.656	8125.659	8126.661	8127.663	8128.666	8129.668	8130.670	8131.673	8132.675				
	Expected m/z	2029.911	2030.162	2030.412	2030.663	2030.913	2031.164	2031.415	2031.665	2031.916	2032.166	2032.417	2032.668	2032.918	2033.169				
	Rel. Abu.	11.090	38.309	71.671	95.204	100.000	87.974	67.170	45.595	27.996	15.754	8.207	3.990	1.823	0.786				
	Rei. Adu.	11.090	36.309	/1.0/1	93.204	100.000	07.974	07.170	43.393	21.990	15.754	6.207	3.990	1.023	0.760				
DP60 -4	Isotopic Mass (da)	9741.180	9742.182	9743.185	9744.187	9745.189	9746,192	9747.194	9748.196	9749.199	9750.201	9751.203	9752.206	9753.208	9754.210	9755,213			
DP60 -4	Singly Charged Ionic Mass	9741.180	9742.182	9743.183	9744.187	9743.189	9745.184	9747.194	9748.196	9749.199	9730.201	9751.203	9752.206	9753.208	9753.203	9753.213			
	27 2	2435.043	2435.294	2435.544	2435.795	2436.046	2436.296	2436.547	2436.797	2437.048		2437.549	2437.800	2438.050	2438.301	2438.551			-
	Expected m/z	5.557	23.035	51.048		97.755	100.000	88.460	69.360	49.071	2437.298 31.746	18.978	10.571	5.524	2438.301	1.273			
	Rel. Abu.	5.557	23.033	51.048	79.675	97.755	100.000	88.400	69.360	49.071	31./46	18.978	10.571	5.524	2.723	1.2/3			
DD70 5	7 (1)	11261 700	11262 711	11262 712	11064.716	11265 710	11266 720	11067 700	11260 725	112/0 727	11270 720	11071 700	11070 704	11070 706	11274 720	11075 741	11076 740		
DP70 -5	Single Channel Lania Mana	11361.708	11362.711	11363.713	11364.715	11365.718	11366.720	11367.722	11368.725	11369.727	11370.729	11371.732	11372.734	11373.736	11374.739	11375.741	11376.743		
	Singly Charged Ionic Mass	11360.701	11361.703	11362.706	11363.708	11364.710	11365.713	11366.715	11367.717	11368.720	11369.722	11370.725	11371.727	11372.729	11373.732	11374.734	11375.736		
	Expected m/z	2272.140	2272.341	2272.541	2272.742	2272.942	2273.143	2273.343	2273.543	2273.744	2273.944	2274.145	2274.345	2274.546	2274.746	2274.947	2275.147		
	Rel. Abu.	2.744	13.270	33.990	60.931	85.458	99.562	100.000	88.803	71.000	51.814	34.883	21.850	12.823	7.091	3.714	1.849		
		400	1005		4000		400		400000	1000					1000	1000	4000		4000
DP80 -:	Isotopic Mass (da)	12982.236	12983.239	12984.241	12985.243	12986.246	12987.248	12988.251	12989.253	12990.255	12991.258	12992.260	12993.262	12994.265	12995.267	12996.269	12997.272	12998.274	12999.276
	Singly Charged Ionic Mass	12981.229	12982.232	12983.234	12984.236	12985.239	12986.241	12987.243	12988.246	12989.248	12990.250	12991.253	12992.255	12993.257	12994.260	12995.262	12996.264	12997.267	12998.269
	Expected m/z	2596.246	2596.446	2596.647	2596.847	2597.048	2597.248	2597.449	2597.649	2597.850	2598.050	2598.251	2598.451	2598.651	2598.852	2599.052	2599.253	2599.453	2599.654
	Rel. Abu.	1.329	7.343	21.343	43.200	68.148	89.023	100.000	99.100	88.256	71.624	53.547	37.199	24.183	14.800	8.569	4.713	2.472	1.240
DP90 -5	Isotopic Mass (da)	14603.767	14604.769	14605.772	14606.774	14607.776	14608.779	14609.781	14610.783	14611.786	14612.788	14613.790	14614.793	14615.795	14616.798	14617.800	14618.802	14619.805	14620.807
	Singly Charged Ionic Mass	14602.760	14603.762	14604.764	14605.767	14606.769	14607.772	14608.774	14609.776	14610.779	14611.781	14612.783	14613.786	14614.788	14615.790	14616.793	14617.795	14618.797	14619.800
	Expected m/z	2920.552	2920.752	2920.953	2921.153	2921.354	2921.554	2921.755	2921.955	2922.156	2922.356	2922.557	2922.757	2922.958	2923.158	2923.359	2923.559	2923.759	2923.960
	Rel. Abu.	3.962	12.885	29.060	50.914	73.674	91.470	100.000	98.087	87.547	71.891	54.795	39.044	26.166	16.575	9.967	5.711	3.129	1.643