

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

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

DP&Charge State		Ions (Above1%)																		
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	-1	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								
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						
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				
		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				
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			
		Singly Charged Ionic Mass	9740.173	9741.175	9742.177	9743.180	9744.182	9745.184	9746.187	9747.189	9748.192	9749.194	9750.196	9751.199	9752.201	9753.203	9754.206			
		Expected m/z	2435.043	2435.294	2435.544	2435.795	2436.046	2436.296	2436.547	2436.797	2437.048	2437.298	2437.549	2437.800	2438.050	2438.301	2438.551			
		Rel. Abu.	5.557	23.035	51.048	79.675	97.755	100.000	88.460	69.360	49.071	31.746	18.978	10.571	5.524	2.723	1.273			
DP70	-5	Isotopic Mass (da)	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		
DP80	-5	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