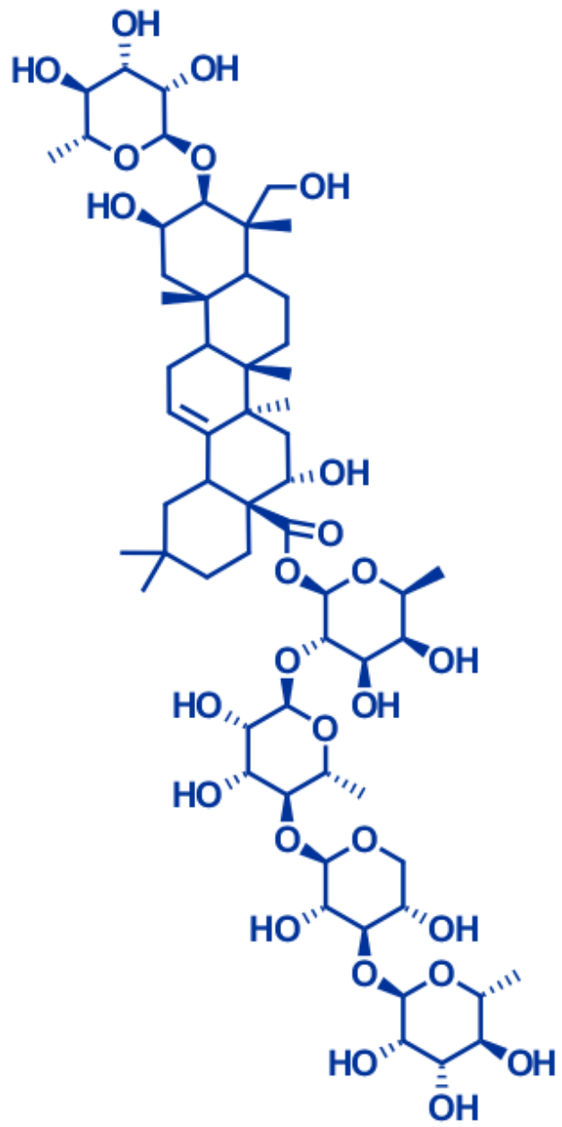
Saponins are Mother Nature's surfactants. Structurally, this class of compounds are glycosides of triterpenes, and their exact masses very often exceed 1000 daltons. If one attempts to analyze higher molecular weight compounds such as saponins, triglycerides, phospholipids, ceramides, or oligopeptides using the default parameters of the Excel Add-In, a message may appear that the mass error window and/or the isotope error window must be tightened. This "window check" is needed to keep the Excel Add-In analysis times under 30 minutes.

Unlike polypeptides, the saponins, triglycerides, phospholipids, and ceramides generally are composed of carbon, hydrogen, and oxygen atoms along with perhaps one nitrogen atom and/or one phosphorus atom. Their possible molecular formulas are very limited. If you are working with these lipophilic compounds, setting the number of nitrogen and phosphorus atoms to 1 or less, and setting the number of sulfur and halogen atoms to zero, will remove this window restriction check. The Excel Add-In will then analyze compounds up to mass 1999 even with error windows set at the maxima.

The spectrum of the week is spectral data of bellissaponin BS1. This compound has an exact mass of 1220.6190. In the DataInput worksheet, the mass error window is set to 5 mDa and the Isotope Error Window is set at 15% absolute. The maximum number of nitrogen and phosphorus atoms were set to 1 and the number of sulfur and halogen atoms were set to zero. The run time was 58 seconds.

All results align the internal 5-carbon xylose residue on the outside of the modular structures, but it is structurally between two deoxymannose residues. In MS-MS, there is a well-documented rearrangement where the internal residue of a trisaccharide is lost (1,2), and this is apparently happening here. The 1089.583 dalton ion cannot be explained any other way.



Bellissaponin BS1

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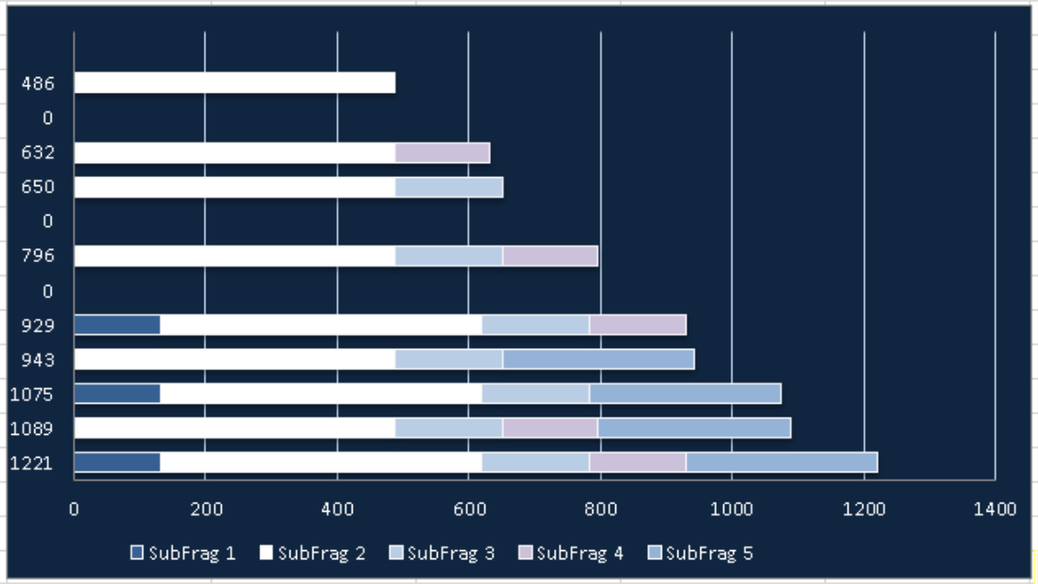
This ms2 (MS/MS) spectrum of bellissaponin BS1 was analyzed with the Excel Add-In. The result for the first partition and highest scoring partition is shown below. This analysis took 58 seconds. (The complete set of partitions can be viewed here: [bellissaponin example]).

Relative Intensities	Neutralized Fragment Masses	Sum of Subfragments
18	486.3345	486.3346
11	614.3818	0.0000
14	632.3924	632.3924
74	650.4030	650.4030
12	760.4398	0.0000
100	796.4609	796.4608
12	906.4977	0.0000
22	928.5031	928.5032
95	942.5188	942.5186
27	1074.5611	1074.5610
37	1088.5761	1088.5764
0	1220.6190	1220.6188



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Alignment of SubFragments

1

Delta	SubFrag 1	SubFrag 2	SubFrag 3	SubFrag 4	SubFrag 5	Σ
	132.0424	486.3346	164.0684	146.0578	292.1156	1221
		486.3346	164.0684	146.0578	292.1156	1089
	132.0424	486.3346	164.0684		292.1156	1075
		486.3346	164.0684		292.1156	943
	132.0424	486.3346	164.0684	146.0578		929
						0
		486.3346	164.0684	146.0578		796
						0
		486.3346	164.0684			650
		486.3346		146.0578		632
						0
		486.3346				486

Partition Score

89

subfragments 5

All Connected to White, but SF5 to SF3

Isotope Ratios	Avg SubFrag MassError	Relative Feasibility					
100 64 25 8							
100 66 27 8	0.09	166	$C_5H_8O_4$	$C_{30}H_{46}O_5$	$C_6H_{12}O_5$	$C_6H_{10}O_4$	$C_{12}H_{20}O_8$	C59H96O26

Sheet1 | Partition (1) | Partition (2) | Partition (3) | Partition (4) | Partition (5) | Partition (6) | DataInput | ...

References

1. Loss of Internal 1 + 6 Substituted Monosaccharide Residues from Underivatized and Per-o-Methylated Trisaccharides, L. P. Briill, W. Heerma, J, Thomas-Oates, and J. Haverkamp. J Am Soc. Mass Spectrom. 1997, 8, 43-49
2. Mass spectrometric glycan rearrangements. Manfred Wuhrer, André M. Deelder, Yuri E.M. van der Burgt. Mass Spectrometry Reviews, Volume30, Issue4, July/August 2011, pages 664-680.

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