

Question 1

Which halogens have these isotopic distributions?

a)



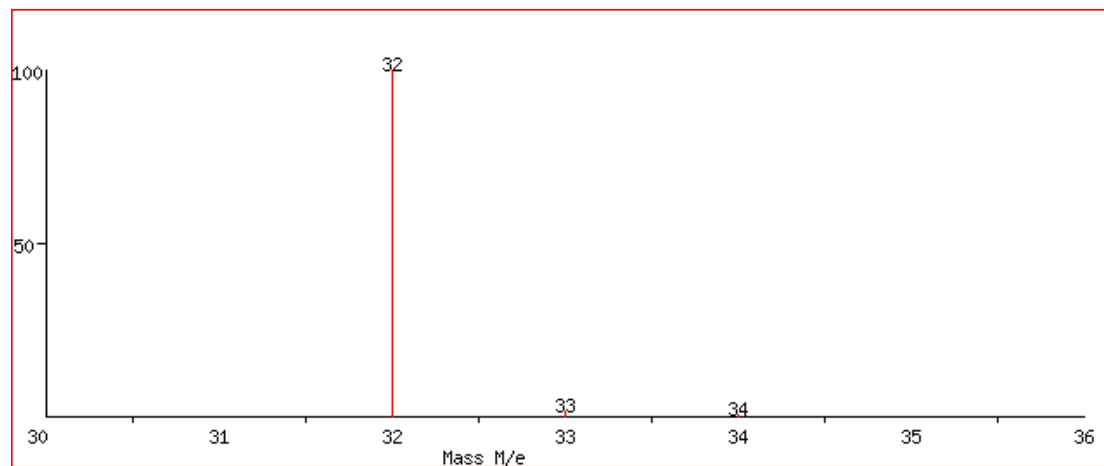
b)



Tip: For additional information go to <http://www.webelements.com/isotopes.html>

Question 2

Which compound has the following MS spectrum?



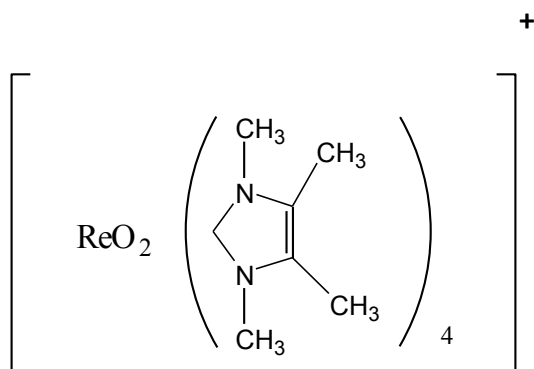
a) CH_4

b) S

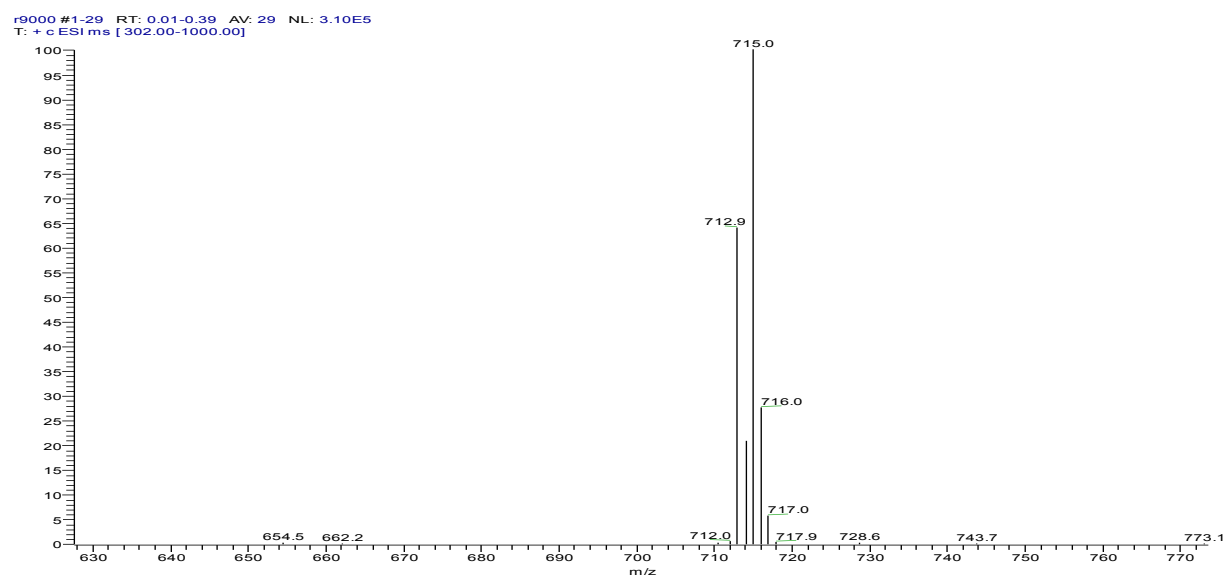
c) CH_4O

Question 3

Consider the following synthesized Re compound (B. Royo, Homogeneous Catalysis Group) with M=715 Da:



Does this ESI-MS spectrum make sense? If so, explain the main peaks.



Tip: Go to <http://www.webelements.com/isotopes.html> and check the isotopic distributions of rhenium.

Question 4

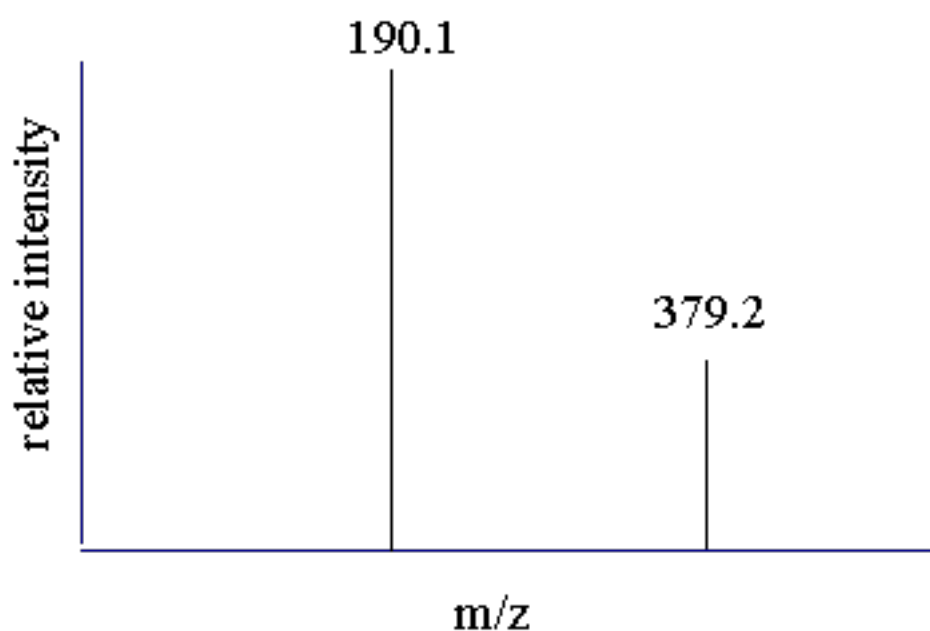
Access the MS spectrum in the file 285_11. Are there any molecular ions containing at least a metal atom? If affirmative, how could you know the identification of this metal? Any clues?

Question 5

Access the MS spectra in the files 44_13B and 413_12. Each spectrum presents a major m/z peak for compounds containing C, N, H and O. Why compounds with the same type of elemental composition present different relative intensity for the isotopic peaks?

Question 6

Determine the mass of the following compound for which the MS spectrum presents two molecular ions with different charge states.



Question 7

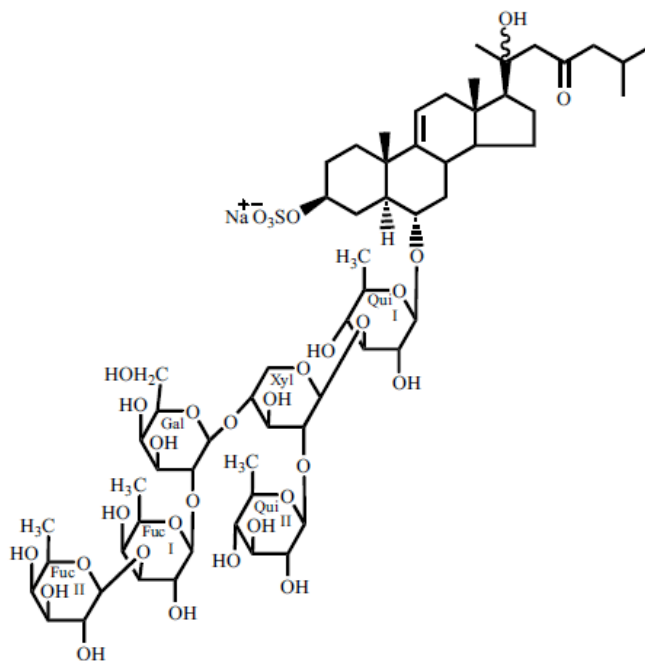
Access the MS spectrum in the file 66_13. Evaluate the charge state of m/z ions 584, 606 and 1167. Could some of these ions correspond to the same compound?

Question 8

Determine the mass of the compound of the file "cytochrome C". Do the deconvolution of the spectrum using the software and confirm the charges attributed with calculations.

Question 9

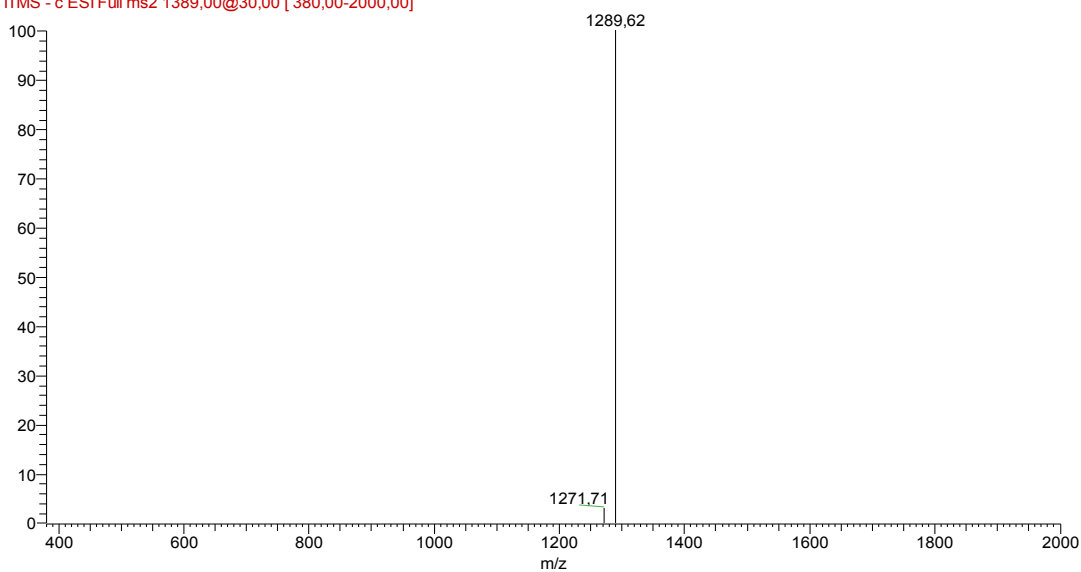
The following molecule (asterosaponin Marthasterosides A, m/z 1379) is composed by a steroidal nucleus, an aliphatic side chain and an oligosaccharide chain (constituted by fucose, quinovose, galactose and xylose).



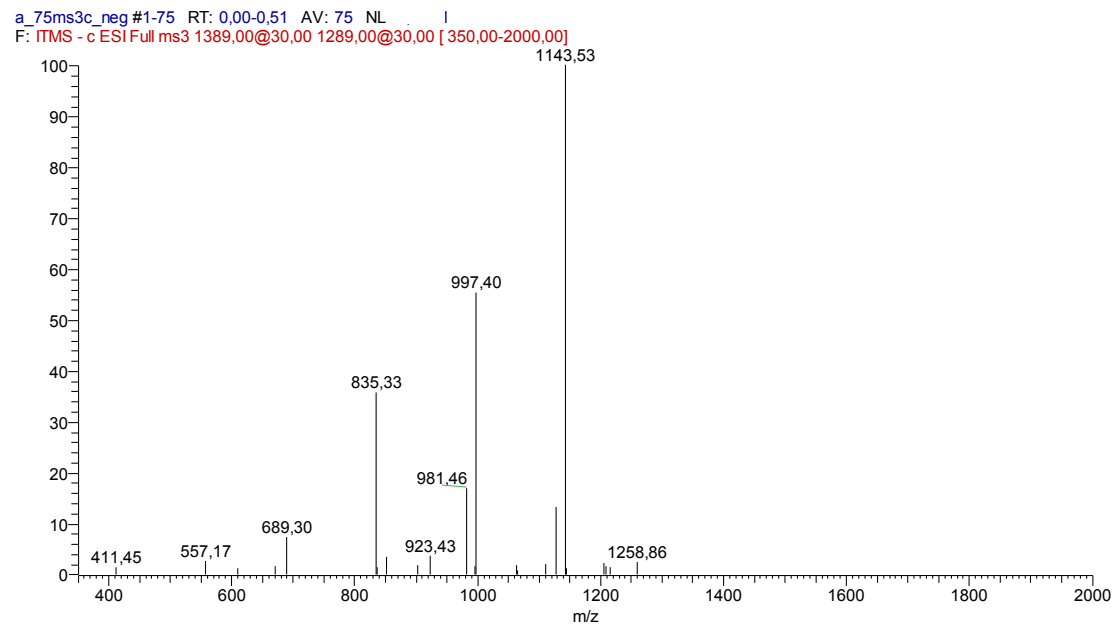
The following MS^n spectra were generated by ESI-MS/MS:

MS^2 spectrum of m/z 1389:

a_75ms2c_neg #3-56 RT: 0.01-0.32 AV: 54 NL
F: ITMS - c ESI Full ms2 1389.00@30.00 [380.00-2000.00]



MS³ spectrum of the MS² fragment at 1289:



Explain the fragment peaks at m/z 1279, m/z 1143, m/z 997 and m/z 835.

Tip: The first fragmentation occurs in the side chain (loss of 100 Da in a retro aldol cleavage). Masses of isomeric quinovose or fucose is 146 Da and of galactose is 162 Da.