Question 1

Which halogens have these isotopic distributions?

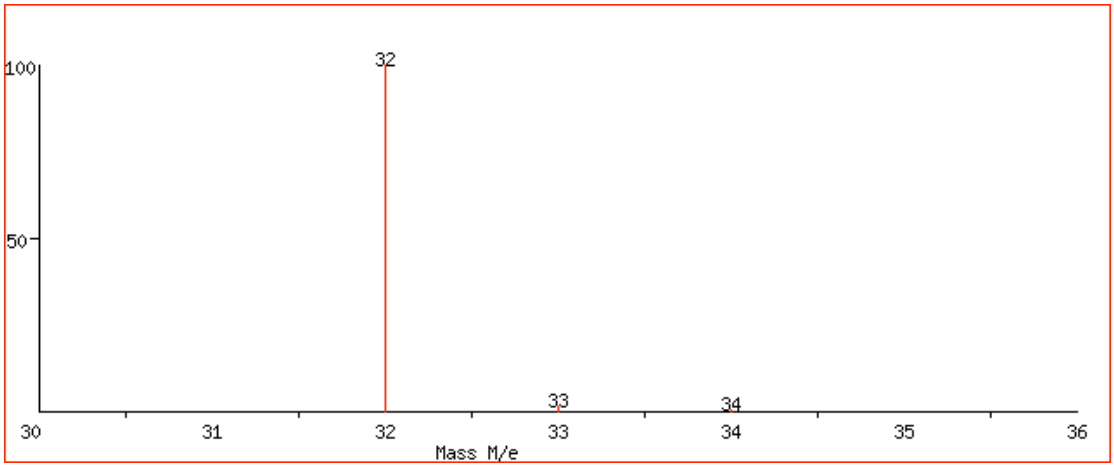
a)

b)

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

Question 2

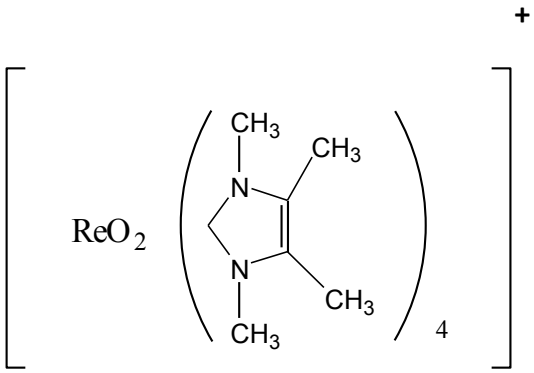
Which compound has the following MS spectrum?



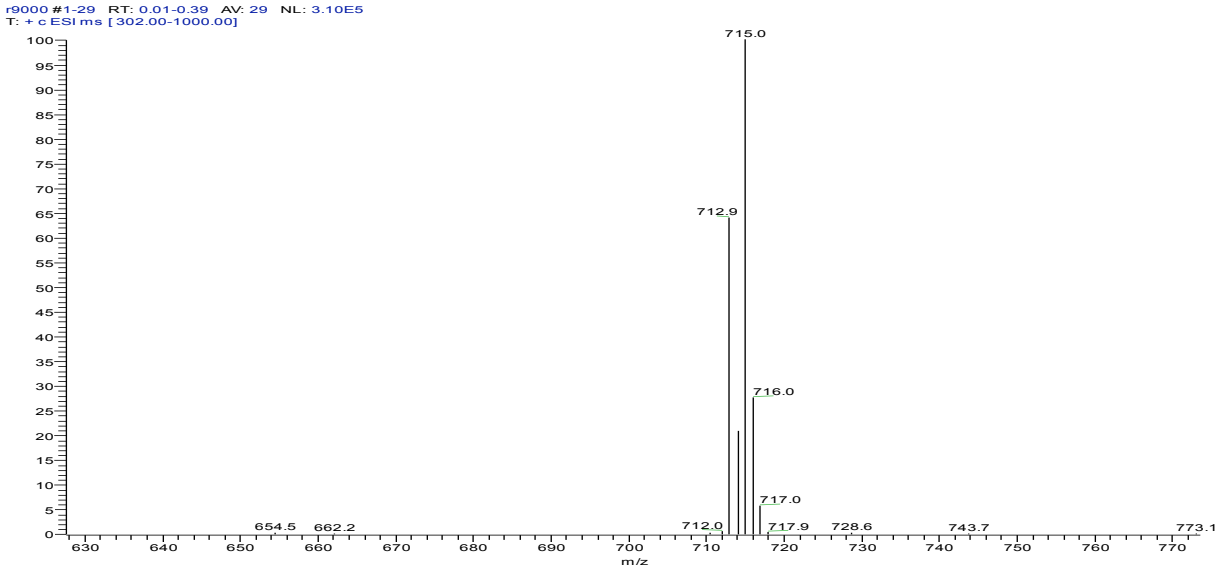
a) CH_4
b) S
c) CH_4O

Question 3

Consider the following synthetized 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 elementar composition present different relative intensity for the isotopic peaks?

Question 6

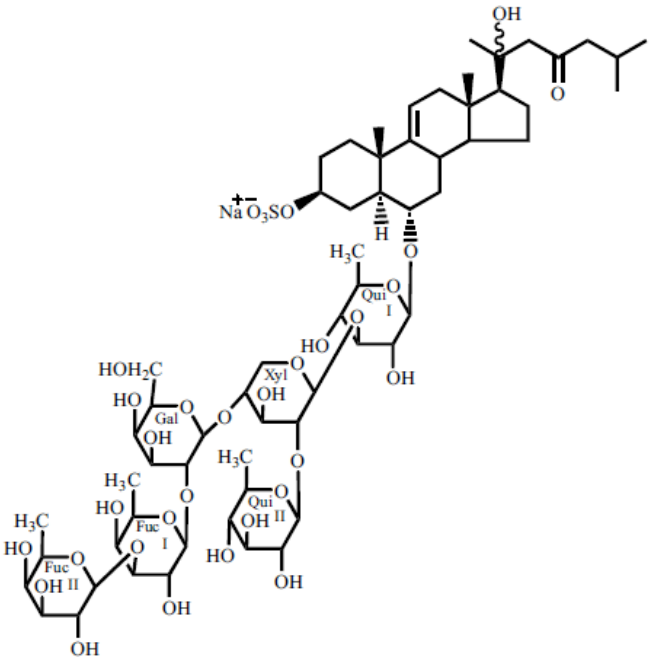
Access the MS spectrum in the file 66_13. Evaluate the charge state of *m/z* ions 584, 606 and 1167. Could some of these ions correspond to the same compound?

Question 7

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.

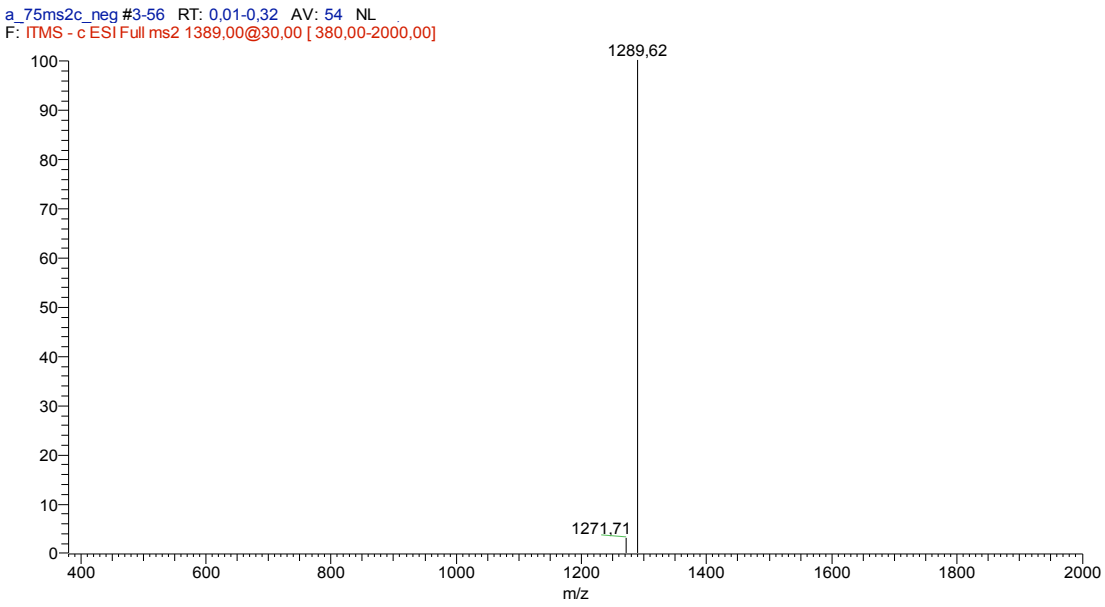
Question 8

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).

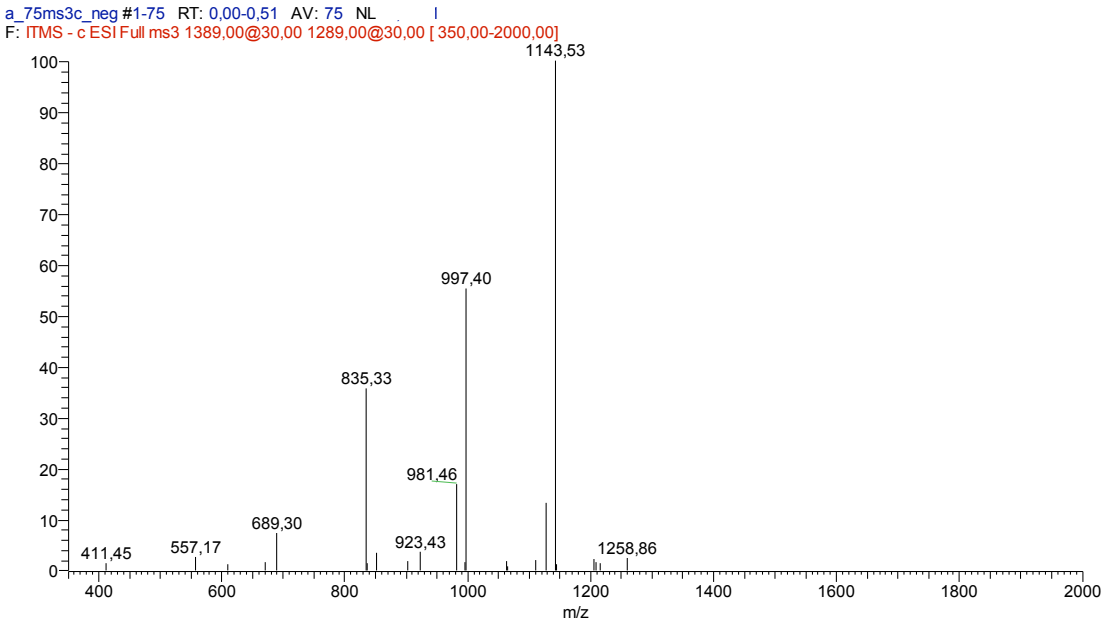


The following MS^n spectra were generated by ESI-MS/MS:

MS^2 spectrum of *m/z* 1389:



MS^3 spectrum of the MS^2 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.