

EPSRC National Mass Spectrometry Service Centre Swansea

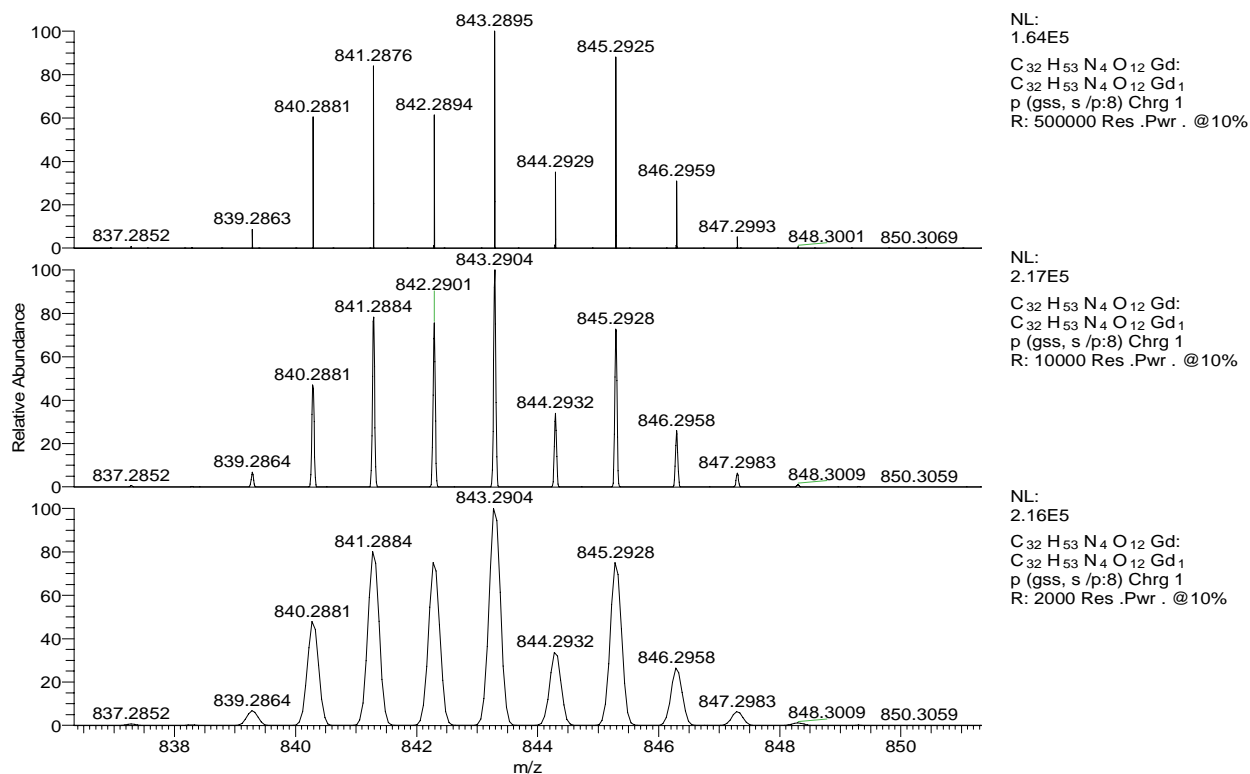
Information Note on:

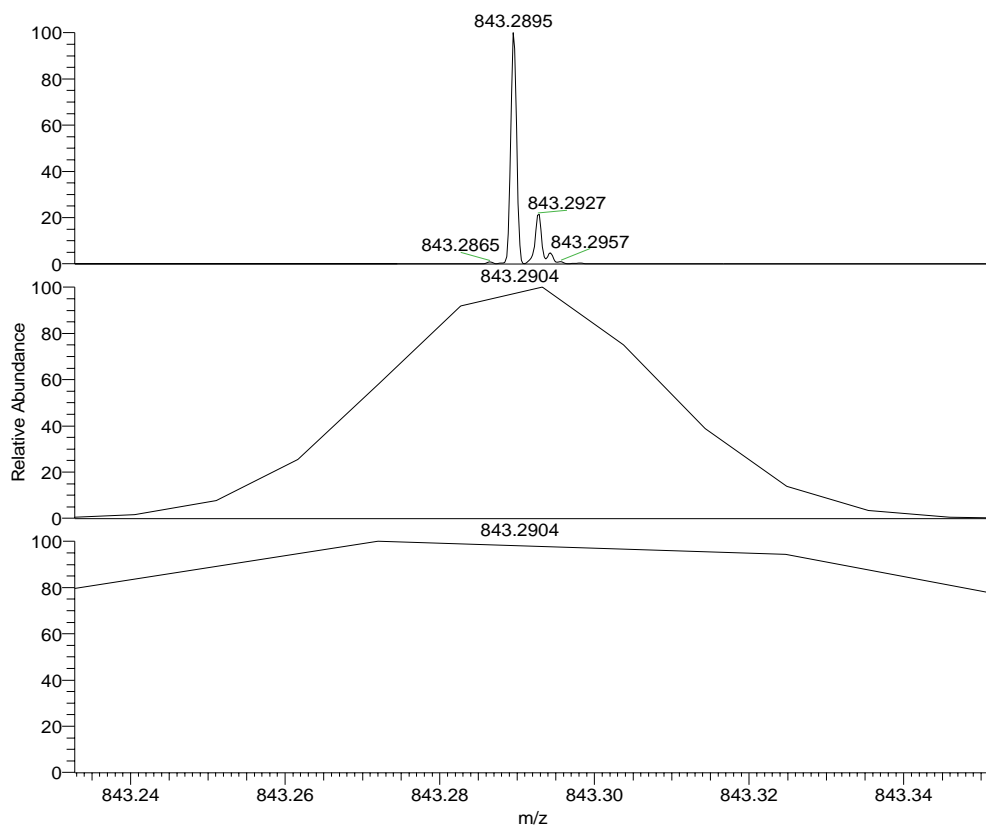
Accurate mass measurement of multi-isotopic species and why the mono-isotopic peak should be selected for accurate mass measurement whenever possible.

When accurate mass measurement is performed on multi-isotopic species, the mass of the lowest mass isotope of the cluster should usually be measured, because this is the only mono-isotopic peak; all other peaks of the cluster are mixtures of different isotope combinations, having the same nominal mass but different exact masses. The figure below illustrates how the apparent mass of the multi-isotopic peaks within the isotope cluster change with mass resolution.

In cases where the intensity of the monoisotopic peak is too low to give adequate ion statistics for reliable measurement, a higher mass peak must be measured even though it is not a pure species. However, in such a case the user of the data needs to be aware of the situation, and the fact that the measured peak is not the mass of a single specie but the average mass of different combinations of isotopes.

For multi-isotopic species, the usefulness for species identification of an accurate mass measurement of a single isotope of a cluster should perhaps be questioned, particularly in light of the above. Compared with, for example, the information given by the isotope patterns themselves of the molecular ion and fragment ion species, the information provided by accurate mass measurement of a single or even a few peaks in an isotopic cluster is relatively uninformative and can be ambiguous. In such cases we therefore recommend that greater emphasis be laid on fragmentation and isotopic information than on accurate mass measurement of a single peak, or even a cluster of such peaks.





NL:
1.64E5
C₃₂H₅₃N₄O₁₂Gd:
C₃₂H₅₃N₄O₁₂Gd₁
p (gss, s /p:8) Chrg 1
R: 500000 Res .Pwr . @10%

NL:
2.17E5
C₃₂H₅₃N₄O₁₂Gd:
C₃₂H₅₃N₄O₁₂Gd₁
p (gss, s /p:8) Chrg 1
R: 10000 Res .Pwr . @10%

NL:
2.16E5
C₃₂H₅₃N₄O₁₂Gd:
C₃₂H₅₃N₄O₁₂Gd₁
p (gss, s /p:8) Chrg 1
R: 2000 Res .Pwr . @10%