

LCT FAQ

Why are there peaks at masses much higher than my expected mass , M?

ESI has a tendency to promote adducts (M+X)+ and dimer and trimers (2MH+ 3MH+ etc) masses. Mass at 2M or 3M are likely these... complicated by adducts.

The most common adducts are + Na (23), + NH₄⁺ (18) and +K⁺ (39). If the MH⁺ ion is in the spectra these ions will appear at +17 + 22 and +38.

Also, a sample concentrated enough to present high abundance "Mers" can present M+ fragment in the molecular weight region. Other adducts frequently seen are plus tfa(114), + CH₃CN (41) lithium (7)+H₂O (18, not to be confused with NH₃ which is way more common) other buffers, salts, chaotropes.

Why don't I see my expected mass?

Is your sample diluted into an electrospray compatible solvent (CH₃CN, MEOH, H₂O, or other POLAR solvents). CH₂Cl₂, HEXANE, Toluene, Acetone are NOT good electrospray solvents. However, as co-solvents in CH₃CN, or DMF, you can get non polar compounds to spray..sometimes and usually as an adduct..

Are you looking for multiply-charged ions? ESI can form ions with more than one charge state. Look for a cluster of ions at 1/2 or even 1/3 of the mass you expect. These are M₂H₂⁺, M₃H₃⁺ etc. These are recognized by the spacing of the isotopomers at 0.5 or 0.33 u.

Spectra dominated by adducts...see above

If your molecule has no unshared electrons, poor proton or cation affinity or only organic acid group(s), it may not work in positive ESI. Try negative ESI if it has an acidic or phenolic groups. The classic technique for aliphatic and aromatic hydrocarbons is EI (or GC-EI). Learn the difference between Electron Ionization (EI) and Electrospray ionization (ESI)

If your molecule is sensitive to protic solvents, water, try CH₃CN, DMF, THF or combinations of these.

I put the vial in the wrong spot and now it won't run samples, how do I fix the problem?

Contact Larry or Bob to fix this problem.

Can I rerun a sample if I do not like the first run?

Yes..We recommend that you rerun the sample under a different file name (and move your sample vial to the proper position in the tray). If you try to overwrite the file, the archived copy will NOT be overwritten and will still contain the original data. You risk losing your new "good run" ...forever.

Contact information:

Call Larry or Bob at 4-3280.

Larry is usually located in B025

Bob is usually found in 3006 or 3007.