

- Each file has 3 composite spectrum plots for each precursor loss composite type, which are all intensity vs. m/z loss (found from subtracting measured m/z from precursor m/z)
 1. Composite spectrum zoomed in around water loss $z=2$ (± 30 bins around theoretical m/z)
 2. Composite spectrum zoomed in around phosphoric acid loss $z=2$ (± 30 bins around theoretical m/z)
 3. Full neutral loss composite spectrum, which measures from m/z of 0 to 100
- Plot details
 - Blue curve is the composite spectrum from the file
 - Red curve is the Gaussian fitted peak – only present if a fit is found for the theoretical m/z
 - Vertical line (orange/green) is at the theoretical m/z of water loss $z=2$ (plot (1)) and phosphoric acid $z=2$ (plot (2)) – orange if the peak is not significant, turns green if the fit is significant (criteria for water $z=2$ is >50 $n_spectra$, for phosphoric_acid $z=2$ is >50 $n_spectra$ and intensity is greater than intensity for water $z=2$)
 - Orange/green shading indicates the extent of the peak, which is how far the algorithm goes out from the theoretical m/z peak to collect other spectra for the Gaussian curve – orange if the peak is not significant, turns green if the fit is significant
 - Blue shading is twice the extent (orange/green shading), which is the range of m/z that the fitting algorithm looks in – only visible if range is within the x-axis range
- Title includes the file name (without .mzML.gz) and the precursor loss composite type, then absolute value of the difference between the phosphoric acid $z=2$ and water loss $z=2$ $\Delta m/z$'s in plots (1) and (2), and the ratio of phosphoric acid $z=2$ intensity to water loss $z=2$ intensity in the fitted peak (red) in plot (2)
 - Absolute difference between $\Delta m/z$'s closer to 0 indicates lower error – and if the fitted peaks are offset from the theoretical m/z (vertical line), this is likely due to absolute calibration offset
 - Intensity ratio is found by measuring the amplitude minus floor of the fitted Gaussian peak for phosphoric acid $z=2$, divided by that for water loss $z=2$