

0.1 List of peak attributes

Whenever we speak of neutral loss we address the neutral loss with the precursor ion.

- **mass**: the m/z value of the peak
- **chemsc**: the sum composition of the peak.
- **frsc**: the sum composition of the fragment. If the peak is a fragment, it is the same as **chemsc**, if it is a neutral loss, it returns the sum composition of the fragment.
- **nlsc**: the sum composition of the neutral loss. If the peak is a neutral loss, it is the same as **chemsc**, if it is a fragment, it returns the sum composition of the neutral loss.
- **frmass**: the mass of the fragment. If the peak is a fragment, it is the same as **mass**, if it is a neutral loss, it returns the mass of the fragment.
- **nlmass**: the mass of the neutral loss. If the peak is a neutral loss, it is the same as **mass**, if it is a fragment, it returns the mass of the neutral loss.
- **errppm**: is the difference between the exact mass and the measured mass in ppm
- **errda**: the error in Da
- **errres**: $= \frac{m}{\text{errda}}$ where m is the peaks mass
- **intensity**: is the list of all intensities through all given samples