






## To Use Deconvolution

Deconvolution is a process that transforms mass spectra from multiply-charged ions into a calculated molecular weight.


### To Deconvolute a Mass Spectrum

This is a generalized procedure; you may need to do some fine tuning.

- 1 In the Data Analysis view, load an electrospray MS data file. The TIC will be displayed.
- 2 Generate the MS spectrum that you want to deconvolute (select the Spectral task tool set and use the spectrum selection tools to pick the spectrum of interest). Note that these operations are performed on data acquired in full scan mode.


- 3  Click the **Enter Deconvolution Tool** button to set up the deconvolution display area.
- 4  When the spectrum is displayed, click the **Find Ions** button to locate masses that will be used in deconvolution.
- 5  Examine the ions that were found. Very noisy data or data with unresolved regions often need special settings to find ions. You can use the **Find Ions Options** button to optimize the set of ions found.
- 6  Click the **Edit Deconvolution Parameters** button to change any of the parameters.
- 7  Click the **Run Deconvolution** button to begin the deconvolution process. Once the deconvolution is done, the Components will be displayed in the upper right window. The Charge States will be displayed in the bottom right window.

- 8 You can look at individual components or groups of components by selecting specific components from the Component list.

- 9  Optionally, click the **Preview Deconvolution Report** button



or click the **Print Report** button.

- 10  Optionally, select components from the Component List box and then click the **Delete Components** button. This action removes the peaks for the selected components from the original spectrum. You can then continue with step 4 above, using this new spectrum.

- 11 Repeat the process.

### Deconvolution Report

The Deconvolution report contains summary information about each component selected, along with detailed information on how each peak in a component contributes to the component's molecular weight. In the first part of the report, the components are ranked by percent relative abundance, which is useful for estimating the percent of impurities.

Note that the actual molecular weight may differ from the computed molecular weight even if the data fit a Gaussian curve perfectly, due to other errors such as errors in mass axis assignment or unresolved chemical impurities.

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The Deconvolution software is optional and is part of the G2720AA Bioanalysis Software package.