

Best Practices for UniDec Deconvolution in MASH Native

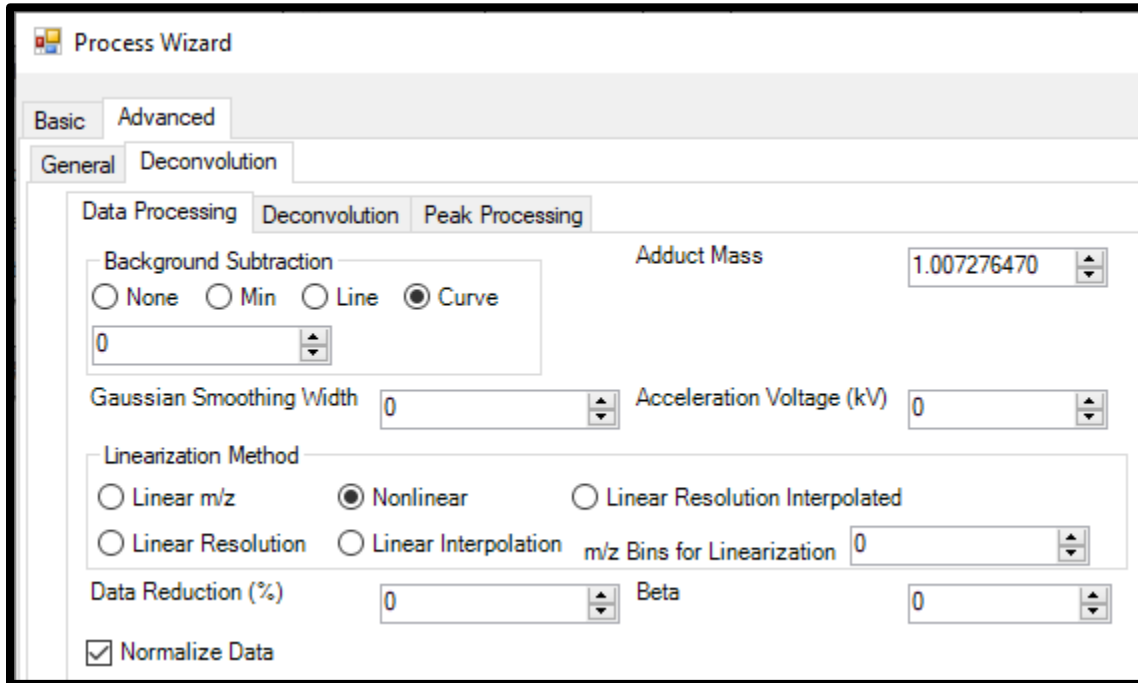
Version 1.1

Introduction

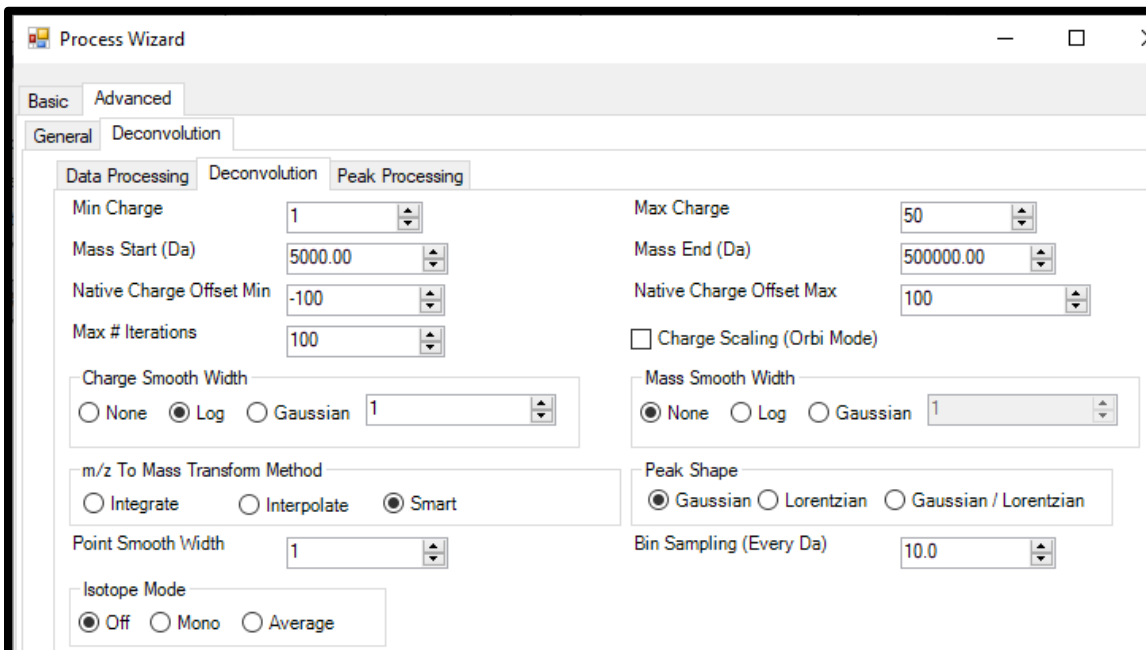
UniDec deconvolution is a powerful tool to perform charge state deconvolution on both native and denatured protein mass spectra. To realize the full potential of UniDec deconvolution, correct selection of parameters is critical. The Marty lab have provided a number of different pre-set deconvolution conditions through MetaUniDec which offer parameter suggestions for UniDec for general applications (default), low resolution native MS, high resolution native MS, and isotopically resolved MS (Kostelic and Marty, 2022).

Suggested parameters when running each deconvolution condition through MASH native are shown with screenshots of the “Data Processing”, “Deconvolution” and “Peak Processing” tabs are show below. For more details regarding UniDec, please see the recent book chapter authored by members of the Marty lab (Kostelic and Marty, 2022). It is important to note that certain parameters influence UniDec deconvolution results and processing time more than others. One such parameter is the “Bin Sampling (Every Da)” in the “Deconvolution” tab. The larger the bin width, the lower the resolution of the deconvoluted spectrum and the faster the deconvolution is completed.

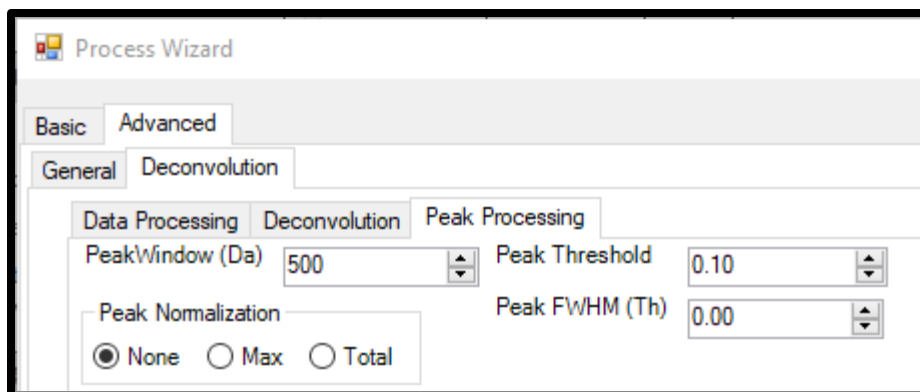
Default Settings for UniDec in MASH Native



Default UniDec deconvolution settings for UniDec data processing in MASH Native.



Default UniDec deconvolution settings for UniDec in MASH Native.



Default UniDec deconvolution Peak Processing settings in MASH Native.

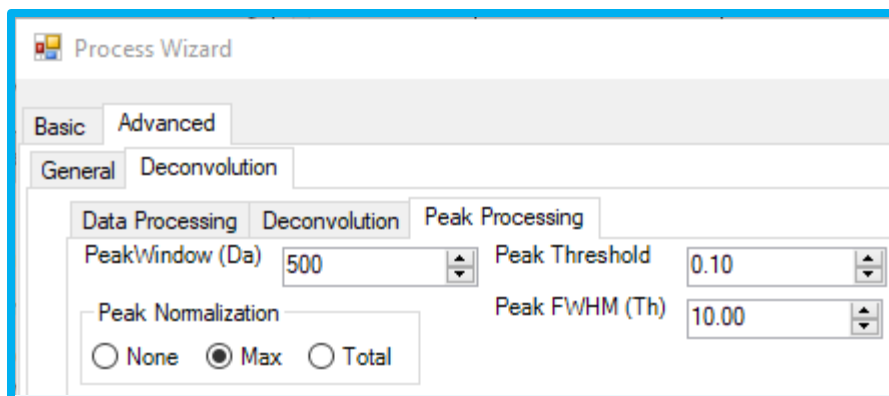
Low-resolution native MS UniDec Parameters

The screenshot shows the 'Process Wizard' window with the 'Advanced' tab selected. Under the 'Deconvolution' sub-tab, the 'Data Processing' section is active. The 'Background Subtraction' section has radio buttons for 'None', 'Min', 'Line', and 'Curve', with 'Curve' selected. A dropdown menu below it shows the value '0'. The 'Adduct Mass' is set to '1.007276470'. The 'Gaussian Smoothing Width' is set to '0'. The 'Acceleration Voltage (kV)' is set to '0'. The 'Linearization Method' section has radio buttons for 'Linear m/z', 'Nonlinear', and 'Linear Resolution Interpolated', with 'Nonlinear' selected. Below it are radio buttons for 'Linear Resolution' and 'Linear Interpolation', and a dropdown for 'm/z Bins for Linearization' set to '1'. The 'Data Reduction (%)' is set to '0'. The 'Beta' is set to '0'. A checkbox for 'Normalize Data' is checked.

Low-resolution Native MS UniDec deconvolution settings for UniDec data processing in MASH Native.

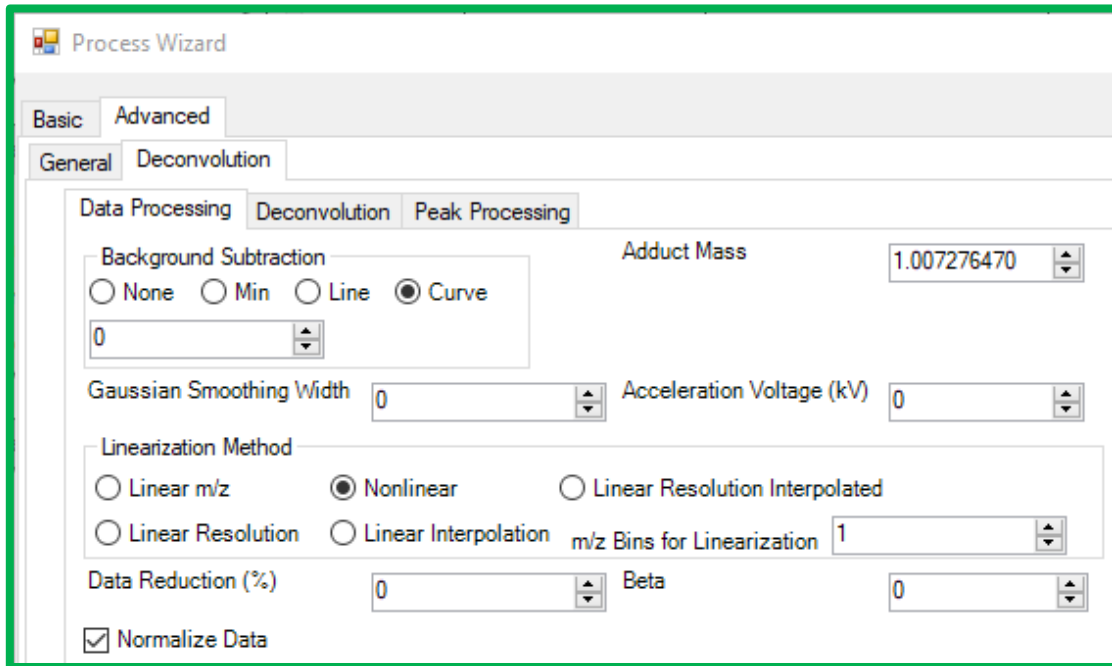
The screenshot shows the 'Process Wizard' window with the 'Advanced' tab selected. Under the 'Deconvolution' sub-tab, the 'Deconvolution' section is active. The 'Min Charge' is set to '1'. The 'Mass Start (Da)' is set to '10000.00'. The 'Native Charge Offset Min' is set to '-1000'. The 'Max # Iterations' is set to '50'. The 'Charge Smooth Width' section has radio buttons for 'None', 'Log', and 'Gaussian', with 'Log' selected. A dropdown menu below it shows the value '1'. The 'Mass Smooth Width' section has radio buttons for 'None', 'Log', and 'Gaussian', with 'None' selected. A dropdown menu below it shows the value '1'. The 'm/z To Mass Transform Method' section has radio buttons for 'Integrate', 'Interpolate', and 'Smart', with 'Smart' selected. The 'Peak Shape' section has radio buttons for 'Gaussian', 'Lorentzian', and 'Gaussian / Lorentzian', with 'Gaussian / Lorentzian' selected. The 'Point Smooth Width' is set to '1'. The 'Bin Sampling (Every Da)' is set to '100.0'. The 'Isotope Mode' section has radio buttons for 'Off', 'Mono', and 'Average', with 'Off' selected. The 'Max Charge' is set to '100'. The 'Mass End (Da)' is set to '1000000.00'. The 'Native Charge Offset Max' is set to '1000'. A checkbox for 'Charge Scaling (Orbi Mode)' is unchecked.

Low-resolution Native MS UniDec deconvolution settings through MASH Native.

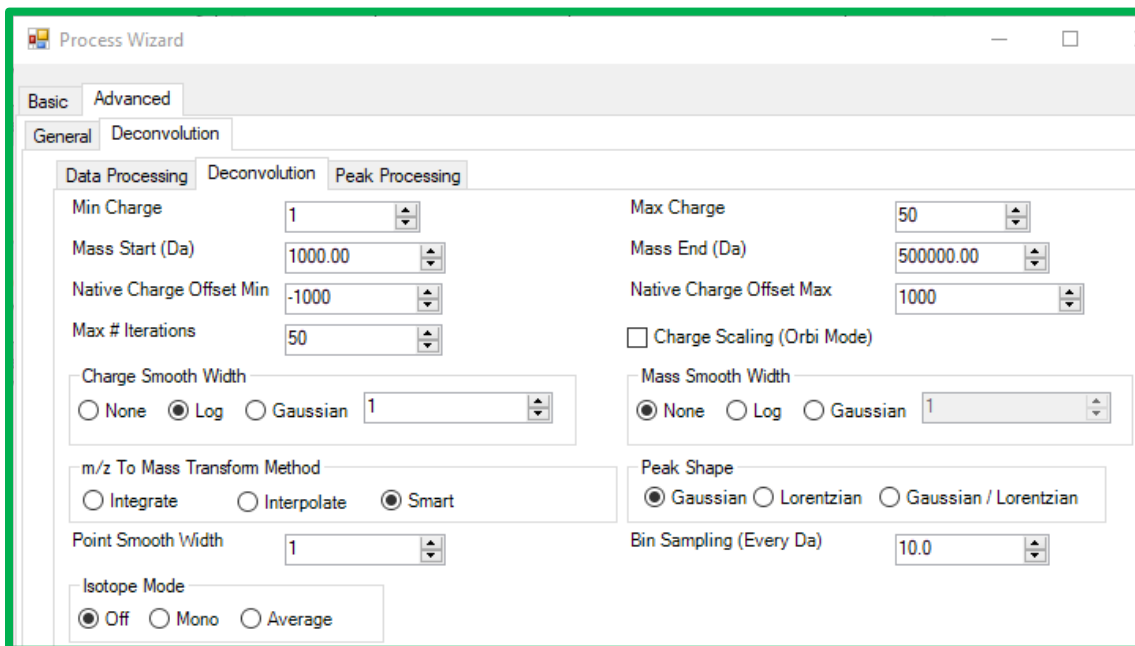


Low-resolution Native MS UniDec deconvolution Peak Processing settings in MASH Native.

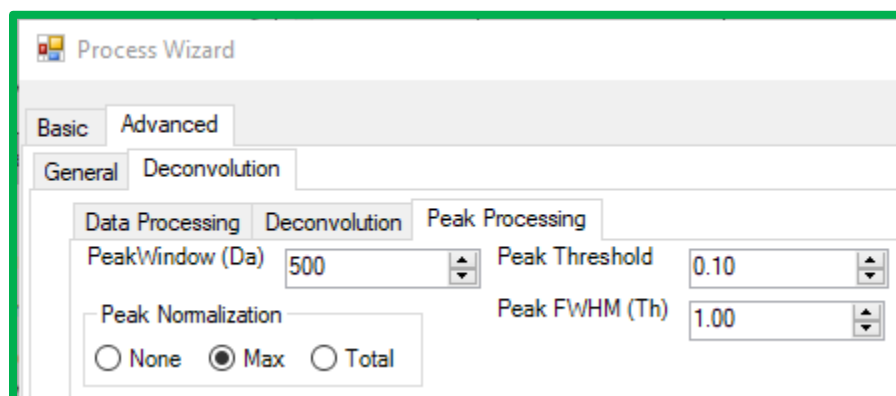
High-resolution native MS UniDec Parameters



High-resolution Native MS UniDec deconvolution settings for UniDec data processing in MASH Native.



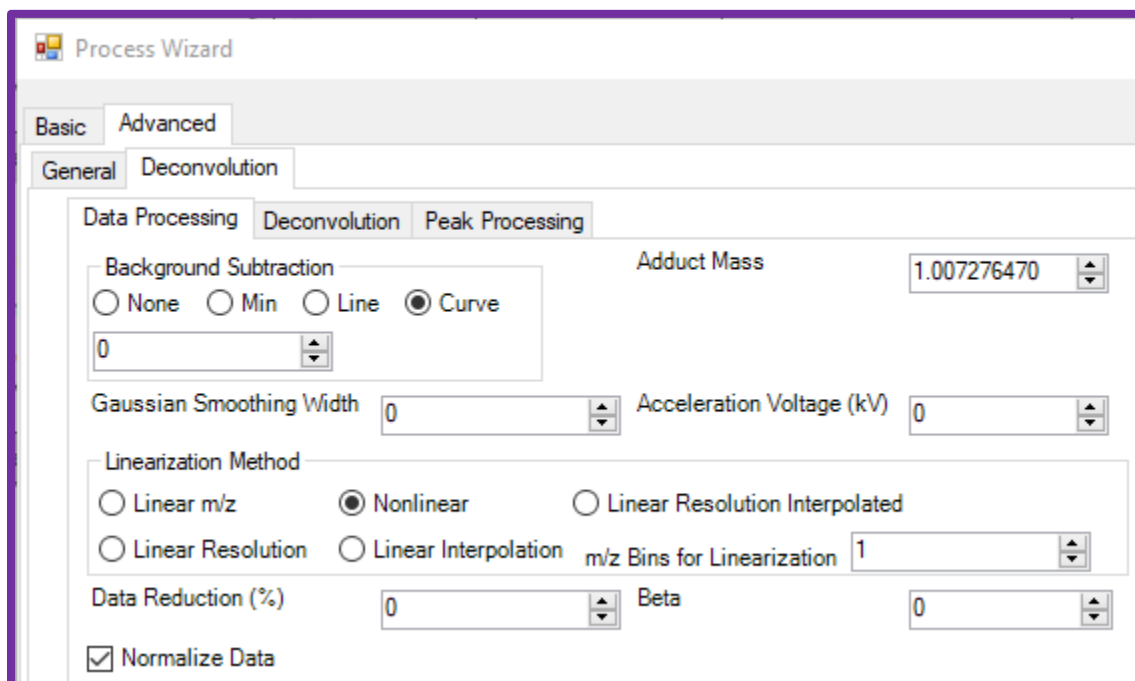
High-resolution Native MS UniDec deconvolution settings through MASH Native.



High-resolution Native MS UniDec deconvolution Peak Processing settings through MASH Native.

Isotopically resolved MS UniDec Parameters

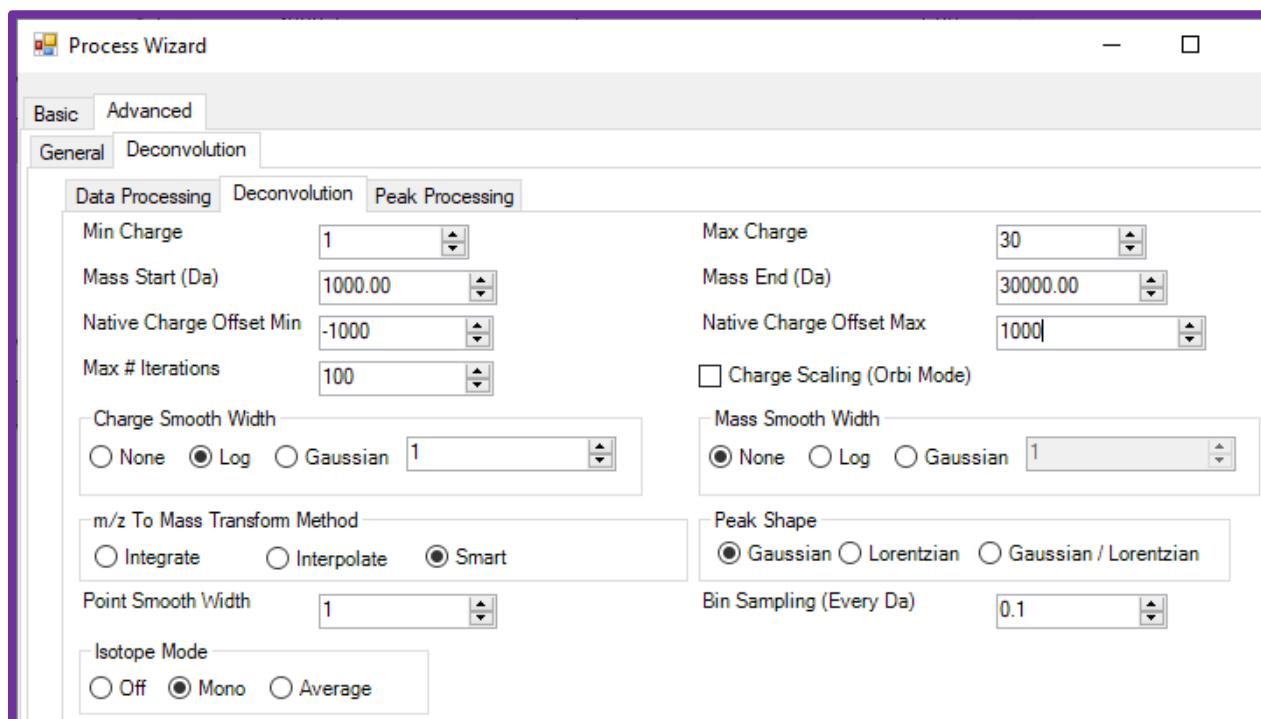
Note: Selection of peak shape parameters in the Deconvolution tab is subject to the mass analyzer used for data acquisition. FTMS and ion trap instruments should use Lorentzian peak shape, while TOF or quadrupole instruments should use Gaussian.



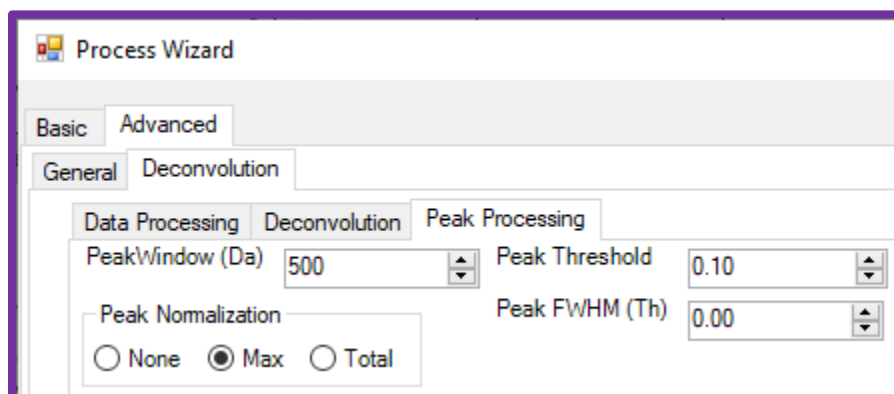
The screenshot shows the 'Process Wizard' window with the 'Deconvolution' tab selected. The 'Deconvolution' sub-tab is active, showing the following settings:

- Background Subtraction:** Radio buttons for None, Min, Line, and Curve (selected). A dropdown menu below shows the value 0.
- Adduct Mass:** A numeric input field with a value of 1.007276470.
- Gaussian Smoothing Width:** A numeric input field with a value of 0.
- Acceleration Voltage (kV):** A numeric input field with a value of 0.
- Linearization Method:** Radio buttons for Linear m/z, Nonlinear (selected), and Linear Resolution Interpolated. Below are radio buttons for Linear Resolution and Linear Interpolation.
- m/z Bins for Linearization:** A numeric input field with a value of 1.
- Data Reduction (%):** A numeric input field with a value of 0.
- Beta:** A numeric input field with a value of 0.
- Normalize Data:** A checked checkbox.

Isotopically resolved MS UniDec deconvolution settings for UniDec data processing through MASH Native.



Isotopically resolved MS UniDec deconvolution settings in MASH Native.



Isotopically resolved MS UniDec deconvolution Peak Processing settings in MASH Native.

References

Kostelic, M.M., and Marty, M.T. (2022). Deconvolving Native and Intact Protein Mass Spectra with UniDec. *Proteoform Identification*, **2500**, 159-180.