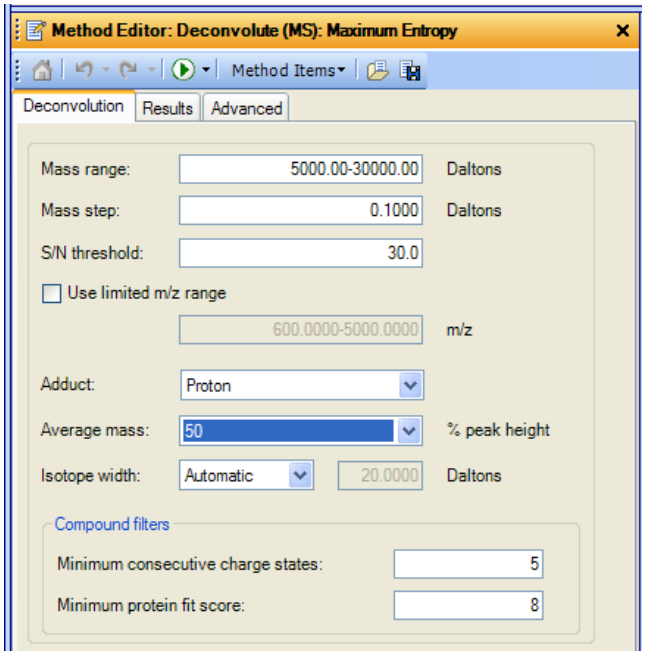
Improvements to the Deconvolution Algorithms in MassHunter Qualitative Analysis rev. B.03.01 Service Pack 3 (SP3)

The new Maximum Entropy algorithm in MassHunter Qualitative Analysis rev. B.03.01 SP3 (Build 346.14) made improvements in deconvolution performance and speed. These have particular applicability when used with data from the 6538/40 UHD Accurate Mass LC/MS Q-TOF models.

How to use Maximum Entropy for high-resolution data

Deconvolute (MS): Maximum Entropy

For high-resolution instruments (G6540A, G6538A) data, if you want to see the isotope resolved deconvoluted spectra for small proteins < 30 kDa, set “Mass step” to be 0.1 Da as the following:



The average mass of the deconvoluted protein is determined and labeled with a red diamond as shown in the figure below. The average mass is also listed in the compound table and is used to match the theoretical value of the target protein.

Maximum Entropy deconvolution result for high-resolution data

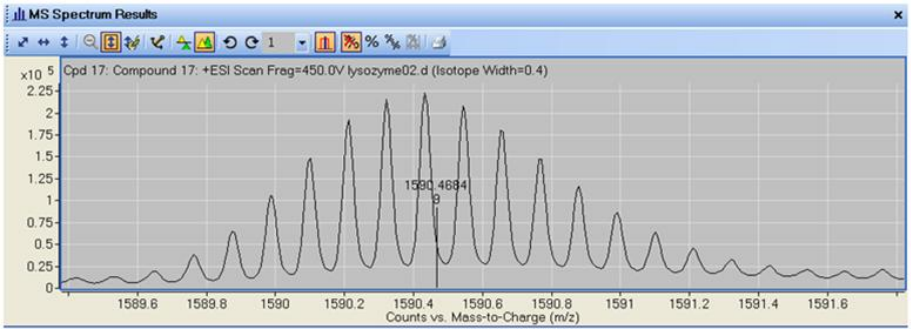


Figure 1. Raw spectrum overlaid with ion sets; 1590.4684 is charge 9 ion's average MW.

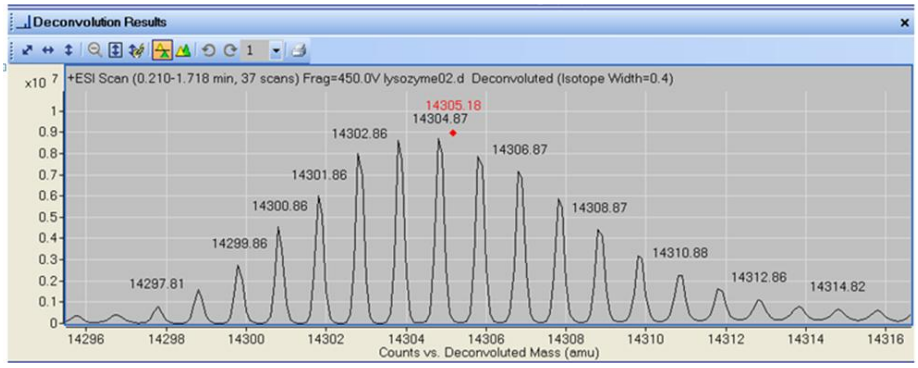
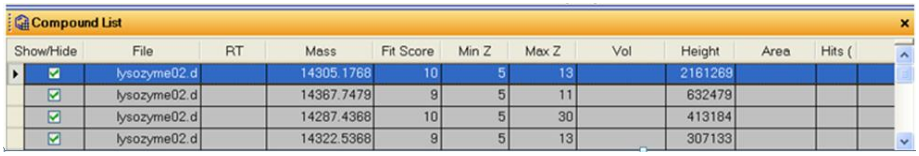


Figure 2. Deconvoluted spectrum—the red label with diamond represents isotope cluster's average MW; Peaks with black labels are isotopes.



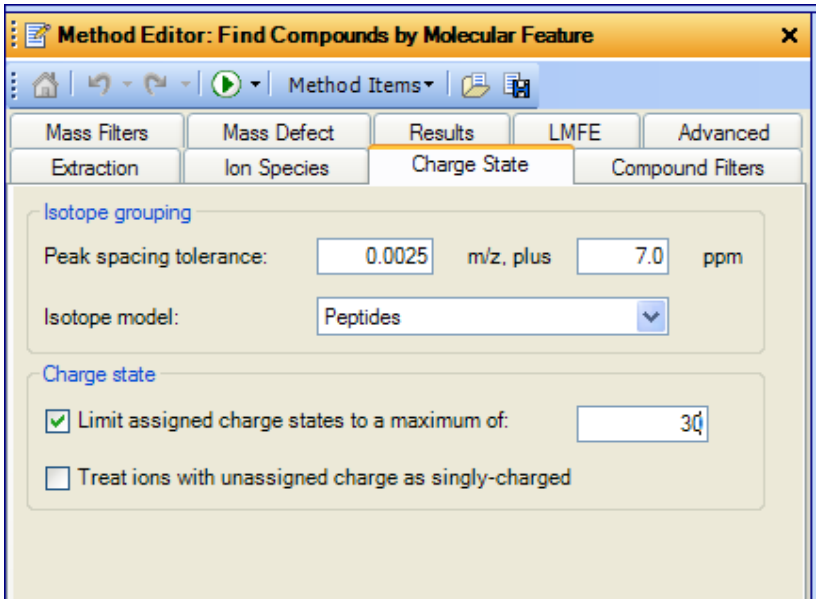
Show/Hide	File	RT	Mass	Fit Score	Min Z	Max Z	Vol	Height	Area	Hits (
☑	lysozyme02.d		14305.1768	10	5	13		2161269		
☑	lysozyme02.d		14367.7479	9	5	11		632479		
☑	lysozyme02.d		14287.4368	10	5	30		413184		
☑	lysozyme02.d		14322.5368	9	5	13		307133		

Figure 3. Compound table—displays protein average MW.

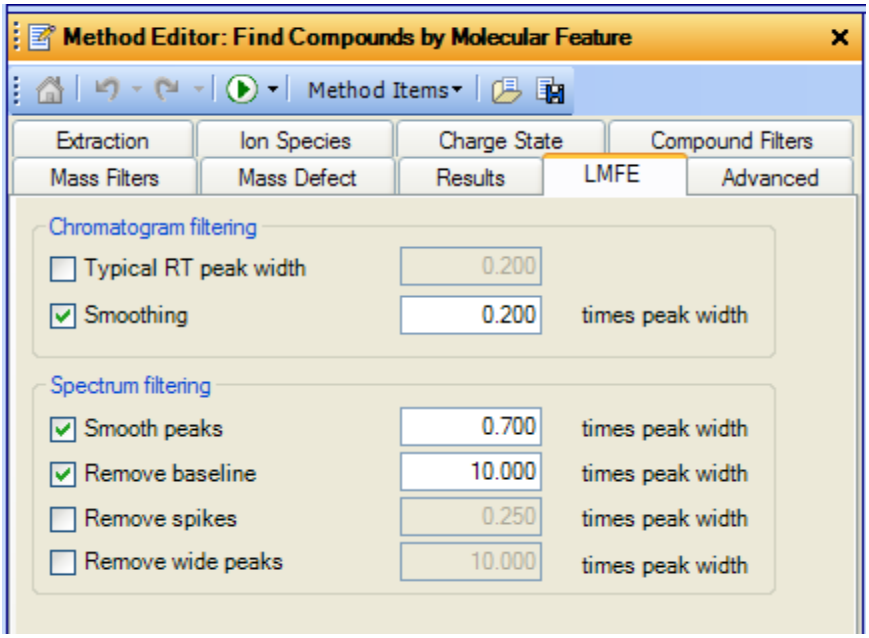
MFE and LMFE

Find Compounds by Molecular Feature

For high-resolution instruments (G6540A, G6538A) data, if you want to obtain the monoisotopic mass for the isotope resolved small proteins < 20 kDa, set maximum charge state to be 30 as the following:



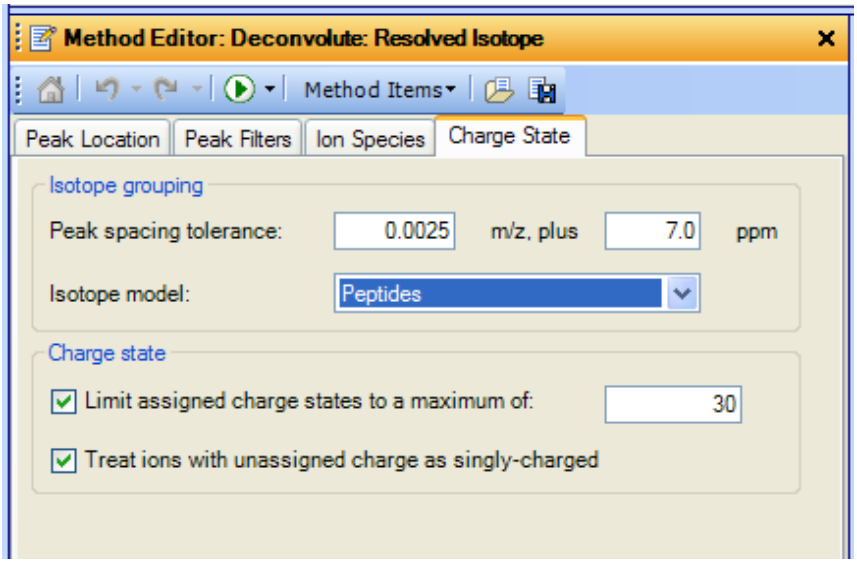
For high-resolution instruments (G6540A, G6538A) data, if you want to use LMFE to obtain the average mass for the proteins, set “Smooth peaks” in Spectrum filtering to be 0.7 times peak width as following:



Resolved Isotope

Deconvolute: Resolved Isotope

For high-resolution instruments (G6540A, G6538A) data, if you want to use Resolved Isotope algorithm for isotope resolved small proteins < 20k Da, set the maximum charge state to be 30 as the following:



Agilent Technologies

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