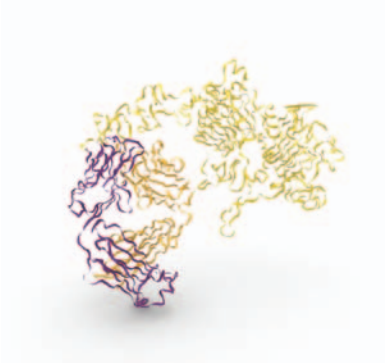
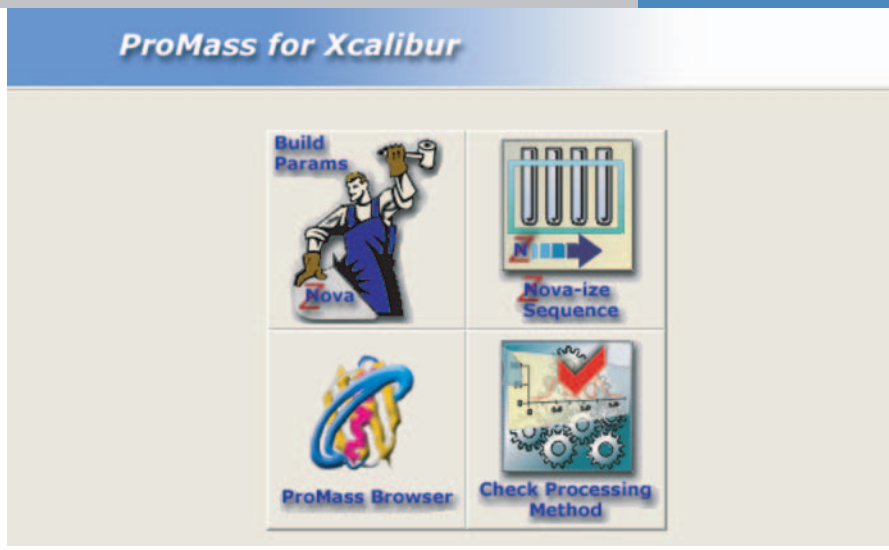
Product Specifications

ProMass Deconvolution 2.5 software is an automated deconvolution and reporting software package for the analysis of intact biomolecules. Users can quickly process ESI/LC/MS data or single ESI mass spectra acquired with Thermo Scientific Xcalibur™ data systems.

ProMass Deconvolution™ 2.5

Applications for Intact Mass Analysis





- Screen for recombinant proteins in complex mixtures
- Confirm molecular masses of peptides and oligonucleotides
- Peptide mapping studies
- Supplement database searches with intact protein mass
- Impurity profiling
- Monitor post-translational, chemical, or drug-target modifications

Powerful but Easy-to-Use Deconvolution Software

An intuitive workflow and simple user interface guides a user step-by-step through the deconvolution process. ProMass uses the novel ZNova™ deconvolution algorithm which produces artifact-free deconvoluted mass spectra, and can be used to process data from a wide variety of biomolecules including peptides, small and large proteins, and oligonucleotides. ProMass does not require high-quality data to produce meaningful results, as it accommodates both low charge-state spectra, and data with a low signal-to-noise ratio.

Deconvolute Complex, Low Signal-to-Noise Spectra

Deconvolution of perfect spectra is simple. Deconvolution of complex spectra is far more difficult. Despite the inherent complexity of the low signal-to noise spectrum in Figure 1, it is easily deconvolved with ProMass to two major components shown in Figure 2.

ZNova is the core algorithm used by ProMass to deconvolute multiply-charged ESI mass spectra. ZNova determines the charge state of every peak in an ESI mass spectrum using ProMass Deconvolution and evaluates all possible charge states for any particular peak as determined by the mass ranges.

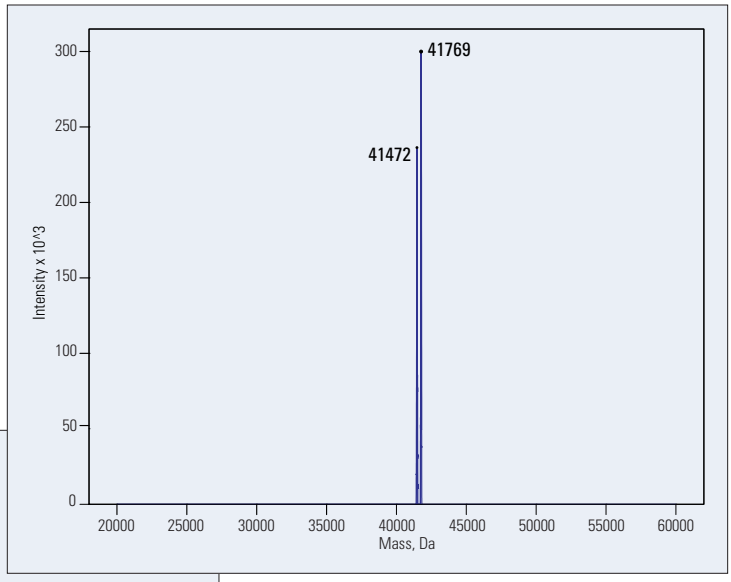


Figure 2: Resolves cleanly into two protein forms

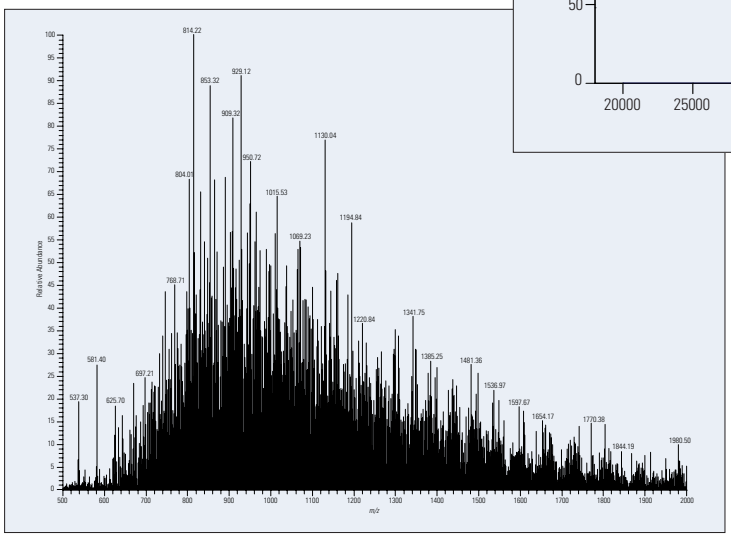


Figure 1: Low signal-to-noise spectrum

Examine, Annotate and Print Spectra

ProMass includes DecView for comparing original and deconvoluted spectra. This interactive viewer allows you to customize viewing and plotting settings, and expand the spectrum to focus on peaks not easily viewable within a web browser environment (Figure 3).

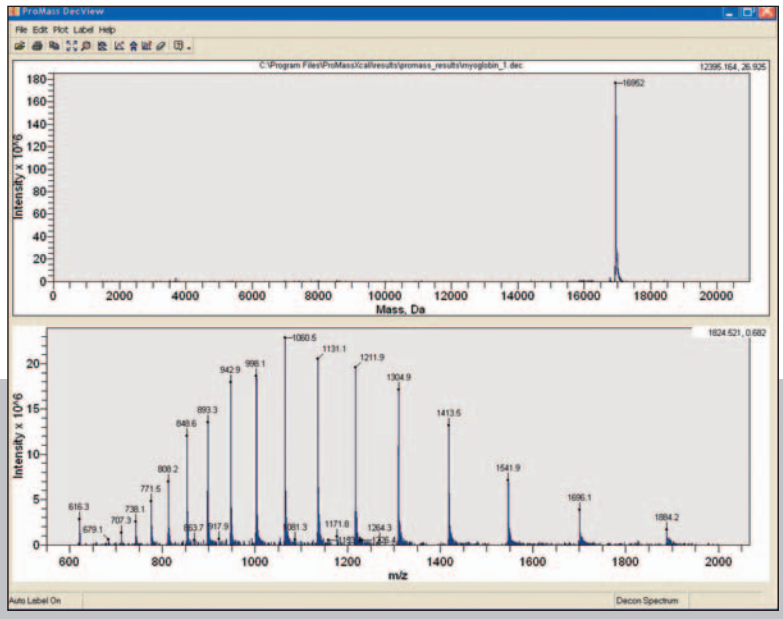


Figure 3: DecView allows you to label, copy, and print the spectra

Intuitive Interface

ProMass is easy to operate. ProMass offers both manual and automated deconvolution modes. The manual deconvolution, shown in Figure 4, is a simple four-step process, allowing the user to get started immediately. Following this four-step process allows users to deconvolute most typical spectra.

Step 1 leads to the menu (inset) which sets the default parameters for step 2. At this point, simply use Xcalibur to copy the spectrum into ProMass.

The customizable output is in an easy-to-use web browser format with a spectrum viewer to check the results.

An advanced menu gives access to a wide range of parameters needed to deconvolve the most difficult spectra. The parameter files can be saved and used for the deconvolution of other spectra.

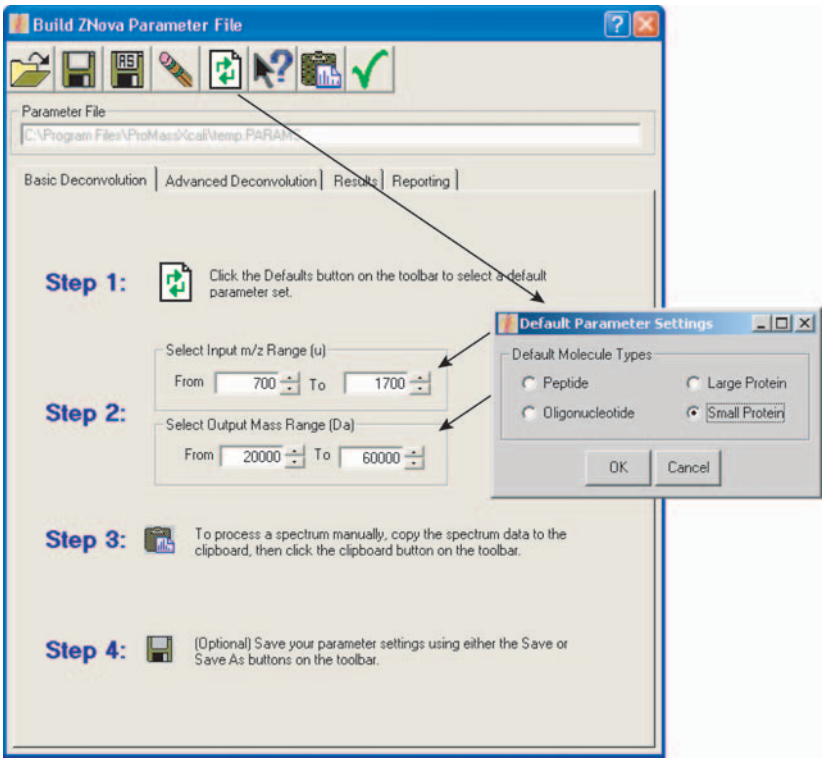


Figure 4: Easy-to-follow interface for Basic Deconvolution

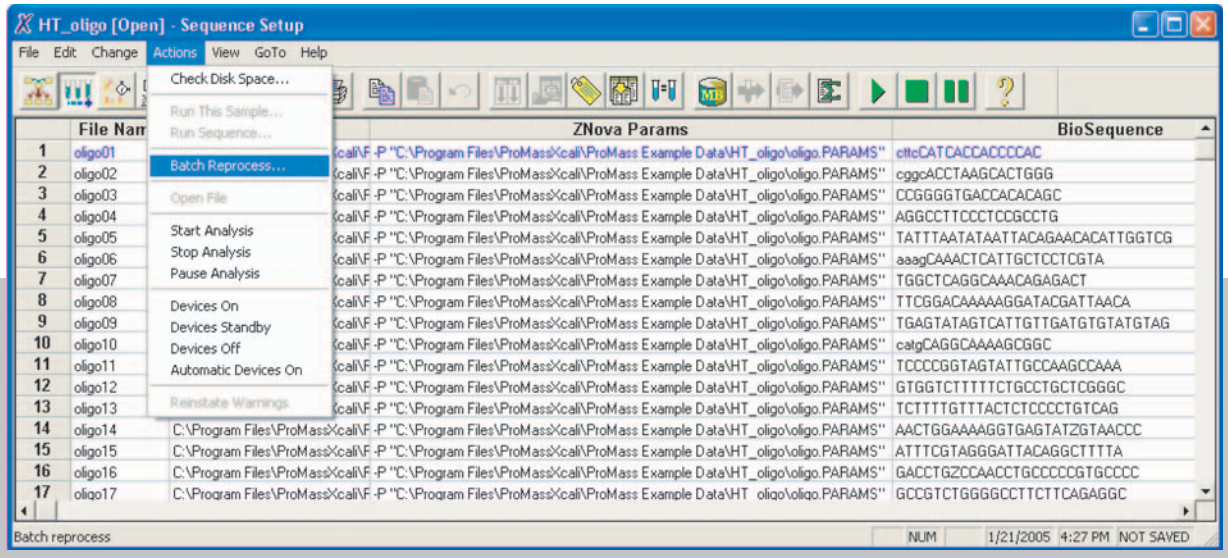


Figure 5: Simplified batch processing of multiple files

High-throughput Capability

ProMass allows users to easily automate their deconvolution analysis. Xcalibur users with existing sequence files can simply click the "ZNova-ize Sequence" button on the ProMass homepage to add ProMass parameters and set up batch processing of data files (Figure 5).

ProMass can also check a processing method (Check Processing Method) to ensure proper performance prior to a "Batch Reprocess".

The batch output comes in a color-coded, interactive visual format as shown below (Figure 6). This data is in HTML format with links to the spectral information.

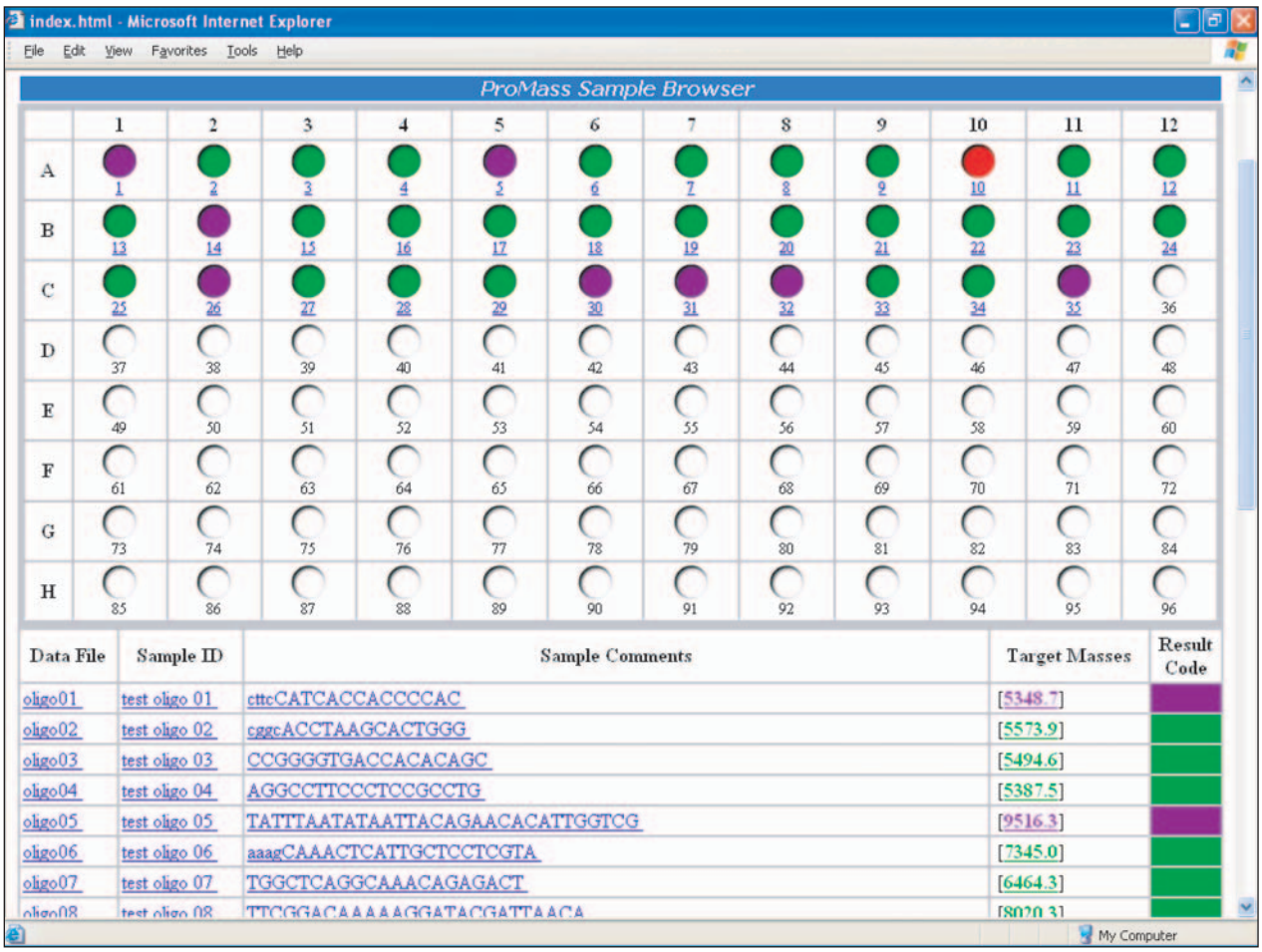


Figure 6: Color-coded results indicate presence and relative abundance of target masses for easy review

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