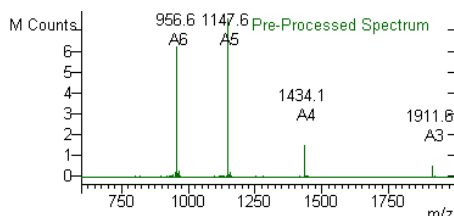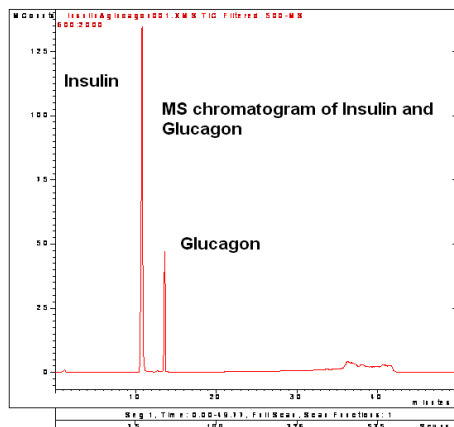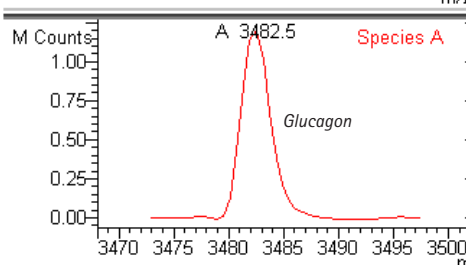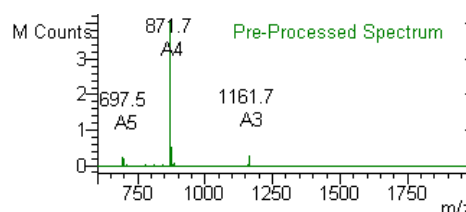# Mass ID™ Software

FOR IDENTIFICATION OF MULTIPLY–CHARGED IONS
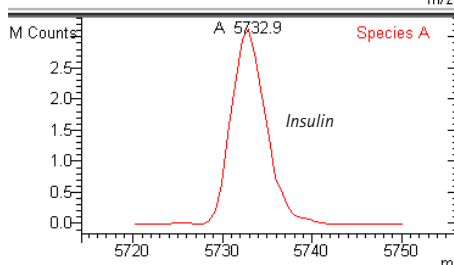
Varian's Mass ID deconvolution software aids in the molecular weight determination of large molecules that are detected as multiply–charged ions, such as proteins, peptides and oligonucleotides.

Deconvolution results of insulin and glucagon mix after chromatographic separation.

Key benefits include:

▶ **"Extended" mass range.** Identify the molecular weight of analytes which are well above the nominal mass range of the instrument.

▶ **Flexibility.** Perform deconvolutions on complex mixtures or single components.

▶ **Utilize multiple data formats.** Process profile spectra from data files (.sms and .xms) or from text files. Works on data from both positive and negative mode collection.

▶ **Spectrum preprocessing.** Apply averaging, smoothing, spike removal and background correction.

▶ **User selectable parameters.** Choose the number of species, type of adducts and mass range to be included in the analysis.

▶ **Convenient data reporting.** Save, export or print deconvoluted spectrum.

NOTICE: This document contains references to Varian. Please note that Varian, Inc. is now part of Agilent Technologies. For more information, go to **www.agilent.com/chem.**

Agilent Technologies

Mass ID™ Software

The Mass ID software is used to process ESI-LC/MS data or ESI-MS spectra acquired on Varian's 500-MS or 300-MS systems. The software performs deconvolution on spectra generated by multiply-charged ions by delivering the appropriate mass for the species as if they were singly charged ions. As a result, the deconvolution software aids in the determination of the molecular weight of large molecules that are detected as multiply-charged ions, such as proteins, peptides, and oligonucleotides.

By executing the deconvolution of these ions, the software "extends" the mass range of the mass spectrometer and identifies the molecular weight of analytes that are well above the mass range of the instrument. The deconvolution results of myoglobin as a single component is shown in Figure 1.
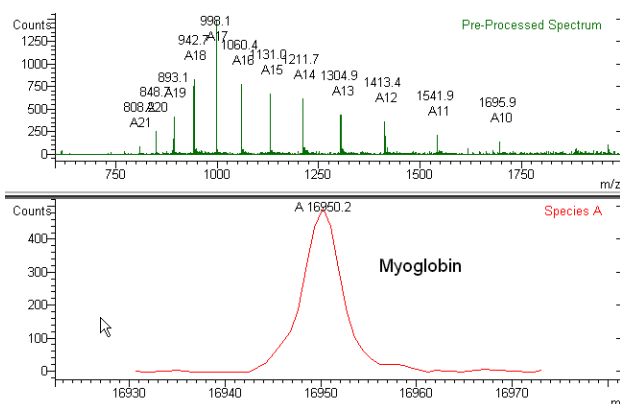
Figure 1 The MS spectrum and deconvolution result of an infused myoglobin sample generated on a 500-MS ion trap mass spectrometer.

In addition to single spectrum deconvolution, the software is also able to perform the deconvolution of infused mixtures or co-eluting components. Figure 2 displays a spectrum generated by infusing a mixture of cytochrome C, myoglobin and bovine serum albumin (BSA) mix into a 500-MS ion trap mass spectrometer. First, the spectrum of the infused mixture underwent spectral deconvolution to separate the three species' individual spectra. In the following step, these spectra were processed to produce molecular weight information on each species. Despite the co-elution, an accurate mass for identification was obtained.
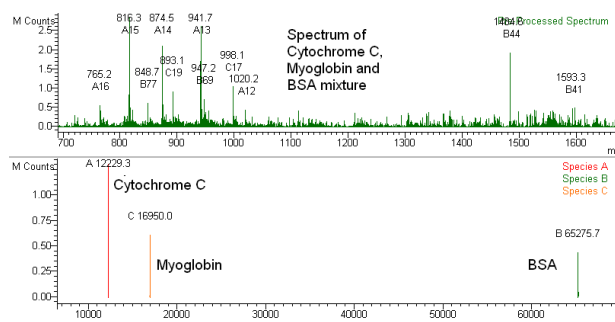
Figure 2 The MS spectrum and deconvolution results of an infused mixture of cytochrome C, myoglobin, and BSA generated on a 500-MS ion trap mass spectrometer.

The deconvolution results for myoglobin as a single analyte or as part of a complex mixture are virtually identical; the masses are 16950.0 as the result from a complex mixture, and 16950.2 as the result from the single component.

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