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Reconstructing Deconvolved Mass Spectra

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Reconstructing Deconvolved Mass Spectra

ABSTRACT

This disclosure describes reconstructing a mass spectrum from a deconvolved mass spectrum.

KEYWORDS

- Mass spectra
- Mass spectrum
- Mass spectrometry
- Mass spectrometer
- Deconvolved
- Reconstructing
- Reconstruction

BACKGROUND

A mass spectrometer is an analytical instrument used to measure the mass-to-charge ratios (m/z) of ions of a sample-under-analysis, or an analyte. Typically, the analyte is separated into components via a chromatographic instrument (e.g., via liquid chromatography, gas chromatography, or capillary electrophoresis), the separated components are introduced into an ion source of the mass spectrometer for ionization, and the resulting ions are subject to transport, confinement, and separation by the components of the mass spectrometer for analysis. The analysis can include generating a mass spectrum depicting a plot of intensity (relative abundance) as a function of the m/z . The mass spectrum is useful for the identification, quantification, and structural elucidation of the sample, for example, peptides, proteins, and related molecules.

Often, the mass spectrum is deconvolved to obtain a list of components (e.g., molecules). However, the deconvolved spectrum might not be reliable.

DESCRIPTION

As described herein, the list of components and the deconvolved mass spectrum can be used to reconstruct the mass spectrum. The reconstructed mass spectrum can then be compared with the deconvolved mass spectrum to evaluate the reliability of the deconvolution.

In more detail, the charge state information of the components identified during the deconvolution of the mass spectrum is used to aid in generating the reconstructed mass spectrum. For example, first a mass spectrum might be deconvolved to generate a deconvolved mass spectrum, and the list of components can be identified from one or both of the mass spectrum or the deconvolved mass spectrum.

Next, the results of the deconvoluted mass spectrum are examined to identify the monoisotopic mass and intensity of the components, and the m/z and intensity of the charge states of each component. For every charge state of each component, the intensity, monoisotopic mass, and an Averaging table is used to generate isotopic profiles in m/z . Figure 1 below shows a schematic representation of the isotopic profiles for three charge states associated with six components identified by a deconvolution.

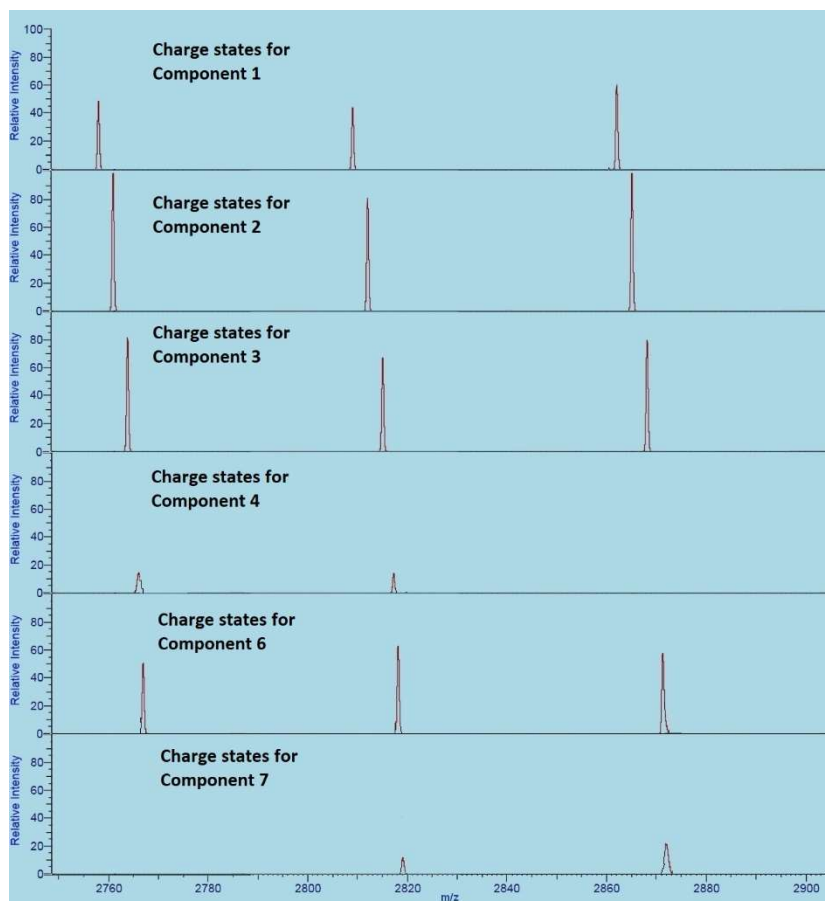


Figure 1

For each possible charge state, the profiles are all added for all of the charge states associated with each of the components identified in the deconvoluted mass spectrum to generate the reconstructed mass spectrum. The reconstructed mass spectrum removes the background, and therefore, provides a direct measure of the magnitude of the background and how much it contributed to the original mass spectrum that was used to generate the deconvoluted mass spectrum.

Because the reconstructed mass spectrum is generated from every one of the charge states associated with each component, it will have a same or similar profile for all charge states. However, the intensity of each charge state is proportional to the sum of the intensities of the components that appeared at that charge state. Thus, the reliability of the deconvoluted mass spectrum can be determined by comparing what is in effect a “copy” of the relevant part of the deconvoluted mass spectrum with the original mass spectrum. Figure 2 below shows a mirror plot depicted the comparison of the original mass spectrum with the reconstructed mass spectrum.

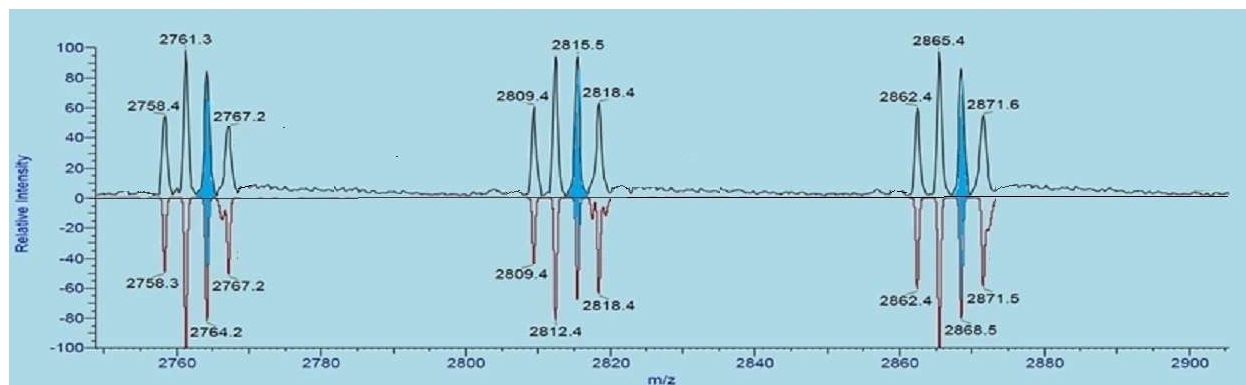


Figure 2

The reconstructed mass spectrum described above differ than reconvoluting a mass spectrum.

Reconvolved spectra can be generated by deconvolving the mass spectrum to produce a set of components, $\{C_i\}$ of mass m_i . Each of these components has a set of m/z peaks, $\{P_{iz}\}$, at charge state Z and m/z value $m_i/Z + m_a$, where m_a is the adduct mass. Next, the technique includes adding the signals for all of the peaks, $\{P_{iz}\}$, to generate a reconvolved spectrum. The signal, $R(x)$ for the reconvolved peak at $x = m_i/Z + m_a$, will be the intensity I_{iz} of peak P_{iz} in accordance with $R(m_i/Z + m_a) = I_{iz}$.

By contrast, reconstructing a mass spectra includes deconvolving the mass spectrum, and then applying a sliding window in mass to identify a set of mass clusters, $\{G_j\}$ in the deconvolved spectrum. For each G_j , determine its mass range, its range of charge states, and total sum intensity, $\sum(I_{iz} \text{ for all } m_i \text{ and } Z \text{ in } G_j)$. For each component, C_i , and Z in G_j , calculate the sum intensity over every peak for this m_i , $\sum(I_{iz} \text{ for this } m_i)$, and over every peak for this Z , $\sum(I_{iz} \text{ for this } Z)$, to generate the signal $S(x)$ for the reconstructed spectrum at $x = m_i/Z + m_a$ in accordance with $S(m_i/Z + m_a) = \sum(I_{iz} \text{ for this } m) * \sum(I_{iz} \text{ for this } Z) / \sum(I_{iz} \text{ for all } m_i \text{ and } Z \text{ in } G_j)$.

Thus, the reconvolved spectrum attempts to recreate part of the original mass spectrum while reconstructed spectrum allows one to compare the results of the deconvolution with charge state clusters in the original mass spectrum.

These techniques can be performed on a chromatography or mass spectrometry system, or using a computing system for post-acquisition analysis.

CONCLUSION

This disclosure describes reconstructing a mass spectrum from a deconvolved mass spectrum. Per the techniques of the disclosure, a reconstructed mass spectrum can be compared with a deconvolved mass spectrum to evaluate the reliability of a deconvolution.