Deriving confidence metrics for automatic peak assignment through n-D Kendrick defect inference networks

Or “Getting software to do the hard work—so you don’t have to!”

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Overview

The data volume produced by Fourier Transform Ion Cyclotron Resonance Mass Spectrometers is an exponential increase, small molecules of complex chemical composition, and their constituent masses provide process feedback and assign automatic peak assignments algorithms to be more effective than manual assignment. Therefore, the development of methods to assist and automate the task of assigning charge states to peaks in mass spectra is a critical process for the high-throughput analysis of complex samples.

Basic Mass Spectrometric Metrics

Basic Mass Spectrometric Metrics are used to provide increased confidence in the assignment of peak identities. All peak intensities in the mass spectra must be within a certain mass error of the library entry. All detected isotopic peaks must exhibit a relative abundance within defined bounds, and all inferred formulae must meet stoichiometric requirements defined by a simple mass-to-charge ratio (m/z) calculation. This metric provides a method to automatically infer the charge state of a peak, but the confidence level one would have in the results would be low. Therefore we apply a threshold to the mass-to-charge ratio to infer the charge state of a peak.

Consistency Metric

The Consistency Metric allows the user to adjust the mass-to-charge ratio threshold used to process a given mass spectrum. This metric can be used to adjust the threshold mass-to-charge ratio to improve the assignment rate of a given mass spectrum.

Uniqueness Metric

The Uniqueness Metric is used to determine the uniqueness of the inferred formulae. The uniqueness metric is used to determine the uniqueness of the inferred formulae. The uniqueness metric is used to determine the uniqueness of the inferred formulae. The uniqueness metric is used to determine the uniqueness of the inferred formulae.

Charge State Deconvolution—With No Isotope Peaks

Removing the charge state of an ion is crucial to being able to assign a formula to it. The mass spectra of complex mass spec datasets are not of the highest quality, and the peaks are often too weak to allow the assignment of a charge state. However, the mass spectra of complex mass spec datasets are not of the highest quality, and the peaks are often too weak to allow the assignment of a charge state. However, the mass spectra of complex mass spec datasets are not of the highest quality, and the peaks are often too weak to allow the assignment of a charge state.

Deconvolution Example—Synthetic Data

A synthetic method was used to deconvolve a n-D Kendrick defect inference networks. This method was used to deconvolve a n-D Kendrick defect inference networks. This method was used to deconvolve a n-D Kendrick defect inference networks. This method was used to deconvolve a n-D Kendrick defect inference networks.

Deconvolution Example—Whisky

The same method was used to deconvolve a n-D Kendrick defect inference networks. This method was used to deconvolve a n-D Kendrick defect inference networks. This method was used to deconvolve a n-D Kendrick defect inference networks. This method was used to deconvolve a n-D Kendrick defect inference networks.

References

[1] E. Hart, J. Timmis, Applied So/g332 Compu/g415ng 2008, 8. 191
[3] TD an/g415gen ac/g415va/g415on
[4] mass spectra—this could greatly improve the rate at which such spectra can be processed.
[5] of peaks in complex mass spectra which allows the peak assignment rate to be greatly improved.
[6] and 
[7] Commonly, 2D KMD plots have proven the most useful, but the approach can be easily extended to higher dimensions if required.
[8] Figure 6: Showing the concept behind the Uniqueness Range.
[9] The same method was used to deconvolve a +ve mode ESI spectrum of malt whisky. Prior