A systematic approach for noise characterization in ESI-Q-TOF spectra

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Motivation

HPLC-MS/MS is increasingly becoming the method of election for large-scale proteomic analysis. The sensitivity of protein identification by peptide sequencing is strongly dependent on the ability to discriminate low intensity peptide signals from the underlying noise. A filtering step preceding peak detection may improve the identification results, but needs a general investigation into the nature of noise and how it can be reduced or filtered. The aim of this work is to develop a systematic approach to characterise and eliminate noise, rather than characterise and detect peaks, as principally proposed in literature.

Methods

A four step approach has been specifically formulated in order to characterise the noise. 1. Acquisition, by mean of an ESI-Q-TOF mass spectrometer, of a dataset of spectra from samples produced ad hoc. This dataset includes a blank run, without peptides, and a set of runs in which only few and known peptides have been placed in the samples. 2. Conversion of the spectra from their original m/z domain back to the time domain (that of the times of flight of ions in the spectrometer). The first domain is ideal for the characterization of the chemical noise, while the second one is more appropriate for the periodic one. 3. Fourier transformation of the m/z spectra in order to find common components of the chemical noise all over the spectra. 4. Fourier transformation of the time spectra in order to find common components of the periodic noise all over the spectra.

Results

The analysis of the spectra of the blank run after Fourier transformation has revealed the existence of components which are present all over the run. Since the blank doesn't contain peptides, these components are clearly typical noise features. Moreover, the same components have also been detected in all of the spectra from the other runs which do not contain peptide peaks. These results suggest that our approach can be used to characterise typical components of the chemical and the periodic noise. The characterization of the features of the noise can be used as the first step for noise detection and rejection.

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