



Engineering Sciences Section – 2005

C46 A Method to Prioritize Differences Between Chromatograms

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The goal of this presentation is to introduce the audience to a new method of identifying the relative order of importance in differences among peaks in the chromatogram.

This presentation will impact the forensic community and/or humanity by demonstrating a case study of the application of the technique to samples analyzed by very high resolution mass spectrometry (Fourier Transform Ion Cyclotron Resonance) is presented.

The talk describes an algorithm for ordering the peaks in a pair of chromatograms in order of importance for determining how different two chromatograms are. The method provides an unbiased measure of the relative importance of peaks for determining differences, which may lead to new insight into the classification of samples.

The algorithm uses the Aitchison metric to measure the difference between two chromatograms by calculating the sum of the log of the ratios of all the peaks. This metric has the desirable property of being strictly monotone decreasing when any peak is removed from both chromatograms. The algorithm orders the peaks to in order of minimum difference in the remainder of the peaks.

An important property of the algorithm is that it scales well to chromatograms with tens of thousands of peaks and therefore can be used as an effective data reduction technique.

A case study of the application of the technique to samples analyzed by very high-resolution mass spectrometry (Fourier Transform Ion Cyclotron Resonance) is presented. This technique produces a very large number of peaks. The samples were chosen for known differences and similarities. Researchers evaluate how the technique performs in ordering the compounds in order of importance for establishing these differences.

Chromatogram, Characterization, Classification