

*ALICE2 for Metabolome** A first step of multivariate analysis: Tea categorization

ALICE2 for Metabolome is an NMR processing software specially developed for metabolome analysis. The software permits comprehensive processing and multivariate analysis for a number of collected NMR data, and so its application to complicated systems with multiple components, such as quality control of foods and materials, is expected. This Note introduces an example of tea categorization.

*ALICE2 for Metabolome is a product of collaboration with Nippon Medical School.

< Sampling and NMR measurements of 176 kinds of tea >

The following 176 kinds of tea were examined: Green tea (Uji, Sayama, Yamanashi-hoji, Chinese etc.), Black tea (Darjeeling, Assam, Chinese, etc.), and Oolong tea (Tieguanyin, Puer, etc.). All the samples were infused at 75°C for 3 minutes, and their centrifugally-separated supernatants were used for ^1H NMR measurements with water suppression.

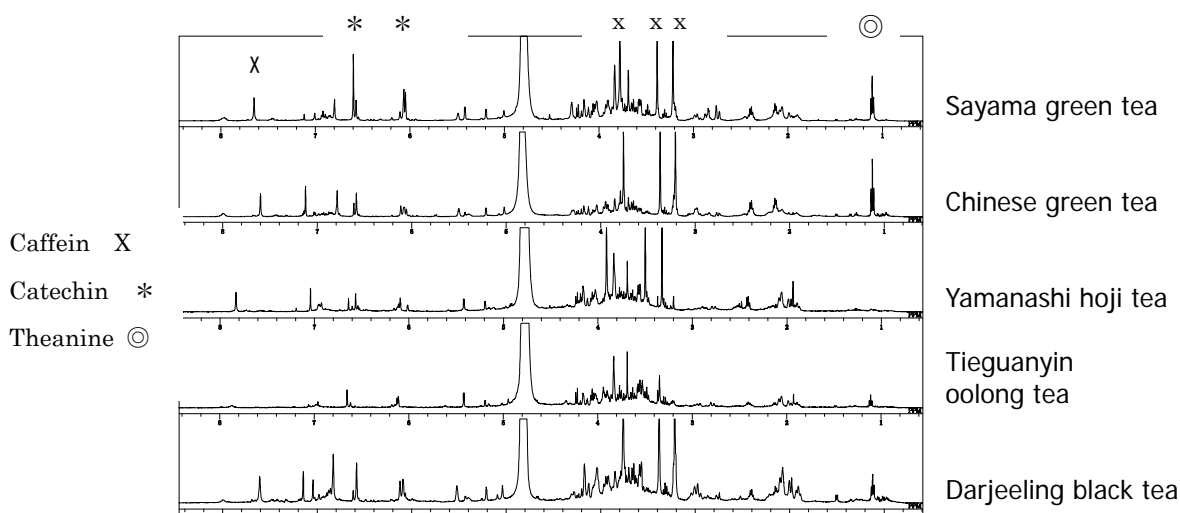


Fig. 1 Typical ^1H spectra of tea (Spectrometer: JNM-ECA500)

Figure 1 shows typical ^1H NMR spectra of tea, where catechin (*), caffeine (X), and theanine (©) exhibit characteristic peaks. However, it is difficult to identify other many constituents, such as amino acids, and only the differences of the spectra are recognized.

< Multivariate analysis using ALICE2 for Metabolome >

ALICE2 for Metabolome processes FID's on the basis of, what we call, Absolute Differential Calculation Method. Each spectrum was segmented into 211 regions of 0.04ppm width, and an integral calculation was performed for each spectral region (bucket integral).

PCA (Principal Component Analysis)

The above processing transforms each spectrum into a single quantity having 211 variables of the bucket integral values, or a single point in the 211 dimensional space; all the NMR data are expressed as 176 points in that space. To extract the characteristics of the data, they are plotted in the principal axes, along which the data are most widely dispersed, as a PCA score plot (Fig. 2).

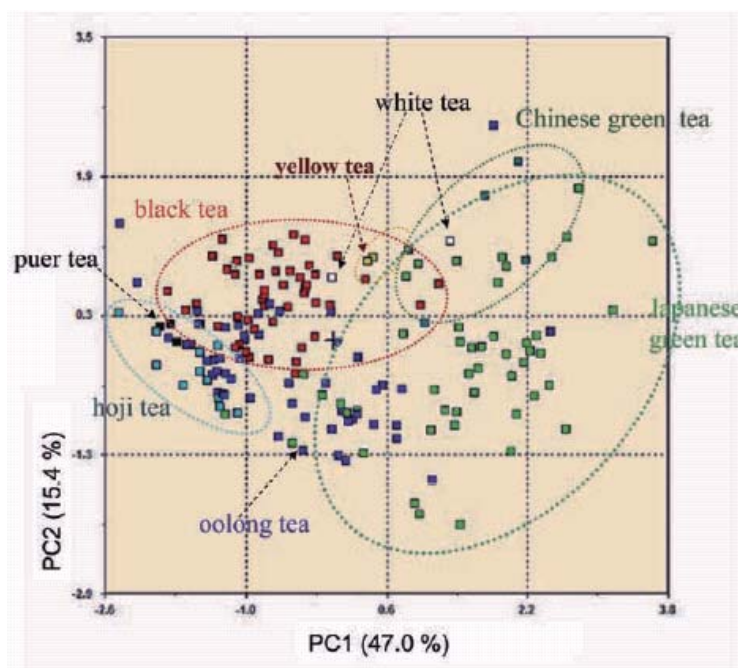


Fig. 2 PCA score plot for the tea samples

PCA score plot in Fig. 2 demonstrates that the data can be fairly well classified into representative tea categories (Japanese green tea, Chinese green tea, black tea, hoji tea, and oolong tea). Also, the score shows that more than 60% of the characteristics of the data are explained by PC1 and PC2.

Discussion

Consider the characteristics extracted by PCA. The main difference of the above tea categories is the degree of fermentation; green tea is non-fermented, black tea is fully fermented, and oolong tea is at various stages of fermentation. The above results may suggest that the degree of fermentation was extracted as the characteristics, leading to tea categorization.

< Conclusion >

Multivariate analysis, more specifically PCA, was applied to ^1H NMR spectra of 176 kinds of tea samples, using ALICE2 for Metabolome. Although the spectra varied depending on the constituents of the samples, PCA could extract characteristics without identifying the individual constituents. PCA as well as SIMCA (Soft Independent Modeling of Class Analogy) is expected to apply to complicated mixture systems having multiple variables.



Multivariate Analysis for ^1H -NMR Spectra of Two Hundred Kinds of Tea in the World
M.Fujiwara, I.Ando and K.Arifuku
Analytical Sciences OCTOBER 2006 , Vol.22 1307-1314