Chemometrics

Application Note

Chemometric Analysis of Soft Drinks

Headspace Mass Spectrometry

Abstract

When soft drinks are volatilized using a headspace analyzer, their mass spectral patterns vary by brand and sweetening agent. Principal component analysis (PCA) of the normalized mass spectra produces scores plots with distinct clusters. These scores plots summarize the similarity and differences among the sample mass spectra.

Samples were drawn from different cans of two primary cola manufacturers. Using the Gerstel Headspace Chemical Sensor, a series of four mL aliquots of beverage were analyzed 30 minutes after opening room-temperature product. No attempt was made to rid the samples of CO_2. The contrast among cola products is unambiguous; both regular colas and their diet counterparts cluster very tightly as shown in a PCA scores plot, Figure 1.
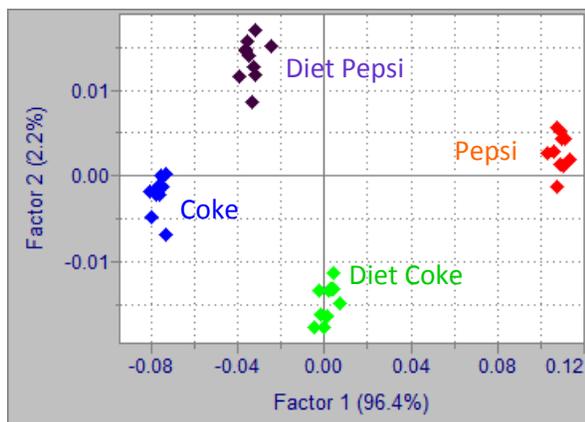

Figure 1. PCA scores of Coca-Cola and Pepsi (both diet and regular)

Four sets of colorless beverages were also analyzed in the same manner. Diet and regular Sprite form distinctive clusters in a PCA scores plot, as shown in Figure 2.
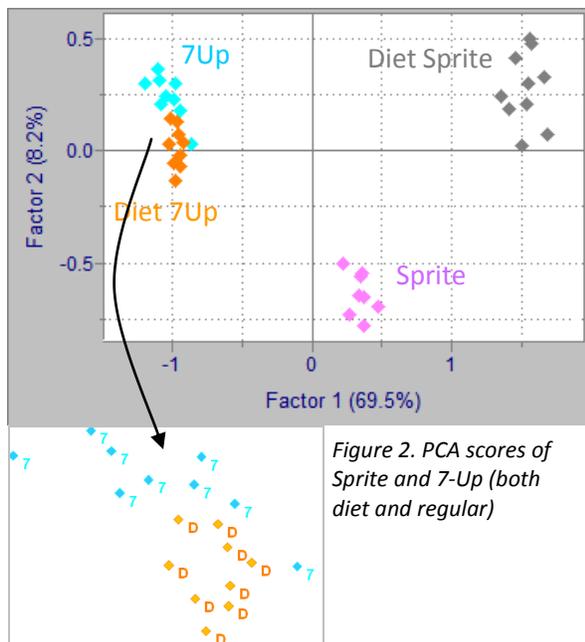

Figure 2. PCA scores of Sprite and 7-Up (both diet and regular)

Diet and regular 7-Up, however, appear to be much more similar to each other, although the two groups can be distinguished (see inset). One explanation: the flavorings (which produce the volatiles signature) in diet and regular 7-Up are comparable.

Figure 3 is a contribution plot which shows differences between regular and Diet Sprite; it may be chemically meaningful. The profiles can be interpreted much like a mass spectrum; using the mass assignments for the two groups, it may be possible to identify specific compounds responsible for their differences.
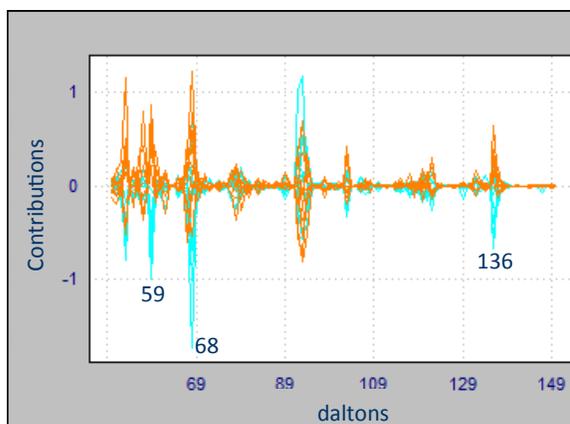

Figure 3. Ions that distinguish diet Sprite from Sprite.

Mass Spectrometer Conditions		
Scan Mode	EI (Atune.u)	
Run Time	0.75 min	
Inlet Temperature	120°C	
Mass Range	46-150 da	
Headspace Conditions		
Temperatures	Oven	80°C
	Loop	85°C
	Transfer line	90°C
Time Events	Heating	20 min
	Interval between samples	4 min
	Pressurize	0.20 min
	Loop fill	0.10 min
	Loop Equil	0.05 min
	Inject	0.30 min
Pressures	Carrier	10 psig
	Vial pressurization	15 psig
Shaking	Low	