

## Application Note

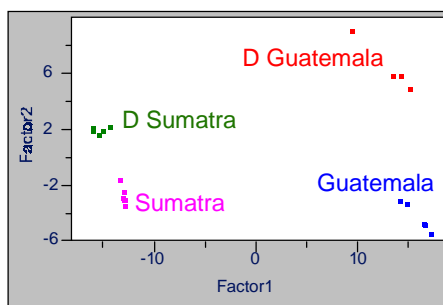
### Headspace Mass Spectrometry

# Analysis of Product Quality Using the HP 4440A

Many products can be classified by compositional differences in their volatile composition. Analysis of such volatiles is compelling because the instruments involved in headspace analysis are simple to operate, they require little maintenance and results are available with rapid turnaround.

The applications described in brief below are examples of headspace analysis by the HP 4440A Chemical Sensor. These eight files are shipped with the instrument and are available as part of the download of Pirouette® from the Infometrix web site.

**Figure 1.** Four different varieties of ground and roasted coffee are easily distinguished by the HP 4440A.



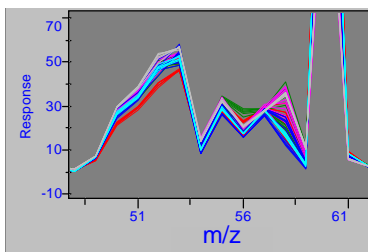
**Java.dat** is an example file that is used in the HP 4440A Primer. This file contains data collected from replicates of four Starbucks coffees: Guatemala and Sumatra, both regular and decaf-caffeinated. The Primer provides a detailed walk-through of the coffee application intended to be a tutorial that can be easily reproduced by an end-use customer.

**Figure 2.** Additional coffee samples along with aged versions and new coffee types are used to show how the system flags unacceptable batches.

Sample	(1-p) value	Match Quality	Coffee Type
Aged DG 1	1.00	No match, closest is:	Decaf Guatemala
Aged DG 2	0.83	Excellent match with:	Decaf Guatemala
Aged DG 3	1.00	No match, closest is:	Decaf Guatemala
Aged DG 4	1.00	No match, closest is:	Decaf Guatemala
Aged DS 1	0.78	Excellent match with:	Decaf Sumatra
Aged DS 2	0.76	Excellent match with:	Decaf Sumatra
Aged DS 3	0.72	Excellent match with:	Decaf Sumatra
Aged S 1	0.66	Excellent match with:	Regular Sumatra
Aged S 2	0.80	Excellent match with:	Regular Sumatra
Aged S 3	0.65	Excellent match with:	Regular Sumatra
Aged G 1	0.97	Good match, with:	Regular Guatemala
Aged G 2	0.93	Excellent match with:	Regular Guatemala
Aged G 3	0.79	Excellent match with:	Regular Guatemala
Ethiopia 1	1.00	No match, closest is:	Regular Sumatra
Ethiopia 2	1.00	No match, closest is:	Regular Sumatra
Ethiopia 3	1.00	No match, closest is:	Regular Sumatra
Ethiopia 4	1.00	No match, closest is:	Regular Sumatra
Ethiopia 5	1.00	No match, closest is:	Regular Sumatra

**MoreJava.dat** continues the training by providing additional coffee samples, some of which are new samples of the Java.dat coffees, some from other parts of the world and some as aged versions of the target coffees. This data set is used in the Primer to show how to automate routine analysis.

**Figure 3.** In a comparison of 10 varieties of Starbucks blends, the distinctiveness of each blend is still evident.



Belaboring the Coffee application, the **Coffee.dat** data set expands the horizons to include 60 samples of 10 different Starbucks roasts. Each of the coffee types can be distinguished from one another by comparing the intensities across the mass range.

