

# Fresh



HUMAN HEALTH | ENVIRONMENTAL HEALTH

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INDIA ANALYTICAL SCIENCES

Dear readers

We are very much proud to inform you that our efforts to reach out to you through this e-FRESH editions has been getting a good response and readership across the country as well as in the other parts of the globe. We are receiving good suggestions and remarks about the content of the news letter which is getting published every month.

So far we have practiced to keep you informed about the new products and technologies from PerkinElmer; as well as the application work carried out at our technology centre in India and overseas by the respective application specialists.

In the present scenario we all look for the quality of the products and the reliable results out of the technology in minimum possible time. This leads to the growing expectations from the industries and regulations for the solutions to the issues related to human and environmental health. PerkinElmer is the one stop solution company for various solutions across the market segments.

This issue consists of the solutions related to the food and beverage industries where various methodologies are being tried for the safer food and drinking water. Similarly we shall be bringing you the technology and applications related to other industries as well in our forthcoming issues for FRESH.

Enjoy reading and send us your comments and business queries.

## WHAT'S Fresh inside...

- High resolution measurement of optical filters in NIR range
- Analysis of tartarates in wine using FTNIR spectrometer
- Automated Thermal Desorber and GCMS for the analysis of VOC
- PerkinElmer Optima ICP 7000 a solution to pharmaceutical sample analysis for inorganic element contents.

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## New range of Thermal Systems to Suit every Analysis



### DSC 4000

Reliable performance, any way you look at it. DSC 4000 - a workhorse performs like a champion. With our DSC 4000, you can expect dependable performance and quality results. This single-furnace, heat flux DSC is designed to run all your routine applications day-in and day-out. Designed with you in mind, this system has an smoothly. Easily upgradeable to a DSC 6000, this instrument can also be fitted with an optional 45-position auto sampler for unattended operation during peak and off-peak hours. Portable cooling device to enhance capability of low temp operations at lower cost of operations.



### DSC8000

Deepen your insights with our exclusive New DSC technology - See what a double-furnace can do for you. With our new DSC 8000 you can expect greater sensitivity and accuracy than you ever thought possible. This double-furnace, power compensation DSC has been redesigned with you in mind. We've improved everything from the furnace design and the lights that illuminate them to the autosampler - giving you fast and reliable results easier than ever before. One look at this instrument will impress you. One look at your data will open your eyes to a world of new opportunity. Take your lab to the next level with our DSC 8000

easy to see why the DSC 6000 is essential for any laboratory.



### DSC8500

Pushing the limits of science - Our hyper-enabled, double-furnace DSC 8500 is truly revealing. We are proud to introduce you to our DSC 8500. This new double-furnace DSC, features our second-generation

HyperDSC® technology. Now you can gain unlimited insight into the structure, properties and performance of your materials and gain the best applications capabilities in the industry. And with our newly designed autosampler, you'll be running samples faster than ever before. Gives you laboratory unlimited potential with our DSC 8500.

Extremely fast controlled scanning rates to 750°C/min for DSC 8500. In-situ ballistic cooling to 1000°C/min, enabling experiments that mimic real-world processes, Extremely fast data



### DSC6000

See what enhanced performance can do for you. DSC 6000 gives you all the advantages of the DSC 4000 and more. Designed for research application, the DSC 6000 comes with Modulated Temperature DSC (MT-DSC) technology for easier data interpretation, and new capabilities for product development and troubleshooting. The DSC can also be fitted with an optional auto sampler and photocalorimetry accessory. It's

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readout rates (100 points/second)  
providing high data integrity

**Typical applications for the DSC  
8500 are as below:**

Characterization of pharmaceutical  
materials  
Polymorph characterization in  
pharmaceuticals  
Process studies in pharmaceuticals  
Process simulation in plastics

## Completing your DSC laboratory solution

All PerkinElmer DSC instruments come with optional autosamplers, so you can perform automated analyses with minimal effort. And with our Pyris™ Player software, setting up a run on one of our autosamplers is simple and quick –and you can run samples during and after business hours. Not sure if you need an autosampler today? Our autosamplers are available as upgrade options to meet the growing demands of your lab.

Pyris software guides you from setup to results Powerful, flexible and proven – the Pyris software platform incorporates sophisticated DSC data

acquisition, analyses and reporting. With a broad range of options, you can grow from very simple routine materials testing to advanced kinetics and research as your requirements demand.



Temperature control options  
Selecting the correct cooling accessory is vital to the performance and applications capabilities of your DSC instrument. We give you a wide range of cooling accessories to suit every cost, temperature and operating expense:

- Chillers
- 2-stage intracooler
- 3-stage intracooler
- Liquid nitrogen cooling system
- Consumables

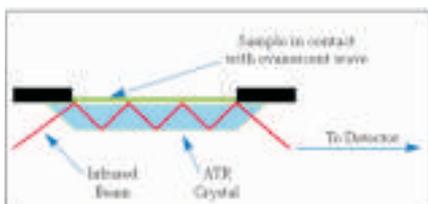
Regardless of form, size or sampling requirement, PerkinElmer's broad range of sample pans and consumables will meet all your application needs. Pan materials include aluminum, platinum, alumina, copper and graphite – available for high and low volumes, high-pressure, solids, liquids and volatile

## How to Eat Food by ATR?

By Purnima Parkhi



The food products like cheese contain high contents of fat. To discriminate it from low content of fat, to analyze other type of dairy products, fast analytical method is Fourier Transform Infrared Spectroscopy (FTIR). Accessory used to analyze these samples is, Horizontal Attenuated Total Reflection (HATR). Throughout 1990's, FTIR spectrophotometers and sample handling accessories became smaller, more robust and easier to use. So,



analysis is much faster. HATR accessory is used for providing spectra of samples that cannot be analyzed by other IR sampling techniques. Then "How to EAT food by ATR"? In

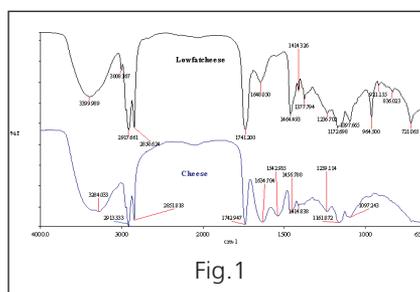


Fig.1

this diet-conscious world, how to differentiate between cheese having higher fat and lower fat? It is very

simple. Just place cheese on a ZnSe crystal of HATR. Scan the samples using infrared radiation and obtain the

spectra. The spectra of a cheese and a low fat cheese are given in Figure1.

As the spectra being correlated become more similar, it is often difficult for operators to determine

whether spectral features are of significance. The interpretation of such spectra has limited the acceptance of infrared spectroscopy, since relatively skilled operators are required. Special Compare function is designed to amplify minute differences in spectra through a series of filters. The filters enhance high signal-to-noise ratio information while minimizing or eliminating variations due to instrumental and atmospheric variations which appear in the spectra. Compare estimates the similarity between two spectra, it emphasizes those features in the spectrum that relate to the chemical composition of the sample, and ignores, or reduces the influence

A correlation of 1.0 indicates that there is a perfect match between the two spectra. In practice this is extremely unlikely, and probably means that the two spectra are copies of the same spectrum. A correlation of zero indicates that the two spectra are wholly unrelated. This is also unlikely because there are almost always some small similarities between spectra.

Cheese with higher fat content (cheese1) is compared to cheese with lower fat content (lowfatcheese03) by using COMPARE software. Correlation value between the two samples 0.8261 proves the discrimination between the two samples. Table I indicates spectrum of Cheese is matching with low fat cheese and there is some difference between spectra of high fat cheese and low fat cheese.

This is very quick identification tool. Correlation value 0.8261 of low fat cheese compared with high fat cheese

indicates that there is certainly some difference.

The bands near 1742, 1239, and 1161 $\text{cm}^{-1}$  in the spectrum of cheese may be assigned to an ester and most likely to a fatty acid ester. The band near 1542  $\text{cm}^{-1}$  is the amide II band from the protein. The band near 1634  $\text{cm}^{-1}$  is partly the amide I band, but is also due to water. The water content is observed by a band at 3284  $\text{cm}^{-1}$ . The bands near 2924 and 2857  $\text{cm}^{-1}$  are due to the methylene stretching

vibrations.

The low fat cheese has a spectrum that is similar in many respects to the high fat cheese.

The water content is higher as can be seen from the strong bands near 1634  $\text{cm}^{-1}$  & 3400  $\text{cm}^{-1}$ , while the protein content appreciably less as shown by the appearance of only a shoulder near 1542  $\text{cm}^{-1}$  ( the amide II band of the protein ).

With the help of advanced software like COMPARE and sampling accessories, FTIR has become more sophisticated technology. Quality of the products can be checked in a very short time and it has achieved consistent authenticity due to algorithms. So to check whether, fat is present or absent in cheese, this is the quick technology. Isn't it very easy to eat food by ATR?

**Table 1**

**Compare Results Table:  
Compare - cheese1.sp**

File:	Correlation:	Factor:	Comments:
cheese1.sp	1.0000	1.0000	Cheese ( Amul ) by HATR accessory.
cheese3.sp	0.9993	0.9712	Cheese ( Amul ) by HATR accessory.
lowfatcheese03.sp	0.8261	0.5200	Amul cheese low fat, low cholesterol.

## Analysis of Acetaldehyde in PET Bottle

### Overview

Acetaldehyde (AA) imparts both taste and odor to bottled liquids. Thus, a key quality issue in the manufacture of PET bottles is the amount of AA created during the manufacturing process. Low AA levels are required by most bottlers. Using the Series 5100, even the highest volume bottle manufacturer can meet the most rigid AA QC testing requirements.

Historically, this critical QC test has involved a large amount of labor to execute the test, lots of paper and then lots of labor to collate and file all of the paper. While the cost of analysis was high, the number of bottles tested was low and the resulting information was saved in a format that was used only in the case of an audit.

The Series 5100 dramatically lowers the per-bottle cost of the test and

automatically combines all results in a useful digital database.

### A Cost Saving QC Tool

The Series 5100 combines a modern sampling system, high sensitivity and a computer architecture into a system that is able to keep pace with the QC requirements of the largest bottle blowers.

Manufacturers who used earlier AA analysis systems see dramatic improvements in the quantity, quality and cost of the analysis. One technician can test more than 700 bottles in a single shift! Most importantly, the information from these 700 bottles is available in a truly useful database format that includes the critical chromatogram required for an audit.

The database information means that the results are a useful QC tool. An audit can now be satisfied in a matter of minutes instead of days. Different factories can easily compare results.

### Bottles per Analysis Run

- Four Models featuring 16, 32, 64 or 96 bottles

### Bottle Sizes

- 0.5 – 3 liters standard
- Smaller and larger sizes possible

### Time per Bottle

- 1 minute

### AA Detection Limit

- 0.1  $\mu\text{g/L}$

### Database Includes

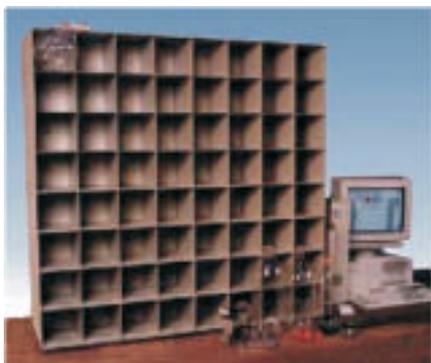
- Full chromatogram
- AA concentration
- Date and time
- Any locally desired information

### Automatic Database Back Up

- System includes Zip drive
- Can choose to go to network

### Typical Extra Saved Information

- Thread split number
- Press and cavity number
- Resin type
- Bottle size
- Re grind %
- Gaylord number



The Model 5164 bottle sampling rack, interface and computer



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## System Description

The Series 5100 is modular and can be ordered with a 16, 32, 64 or 96 position testing rack. Field upgrades to a larger option are possible. The following items are included in the analyzer:

- Bottle sampling rack
- Modified gas chromatograph
- Vacuum pump
- Computer to sampling rack interface
- Computer and printer

Figure 2 presents a simplified plumbing diagram of a 16 position analyzer. The analyzer uses two parallel sampling paths. The analysis cycle time is just under two minutes. Because two bottles are analyzed at the same time, the effective analysis rate is 1 bottle per minute.

An important feature in all parts of the sampling system is the use of very large porting on the various valves and straight, large ID tubing. The result of these construction techniques is the fastest possible equilibration and evacuation times. Compared to earlier systems that use 16-position rotary stream selection valves, the number of bottles tested increases, detection limits are optimized and sample carryover is minimized.

## How It Works

After the system is mechanically installed, the first step is to customize the provided example database. The database is customized to include the details that will be saved with each preform record. Some typical information is press number, cavity number, thread splits, resin type, bottle size and so forth. Every piece of information to be saved with the AA concentration and chromatogram is entered. The database also includes a

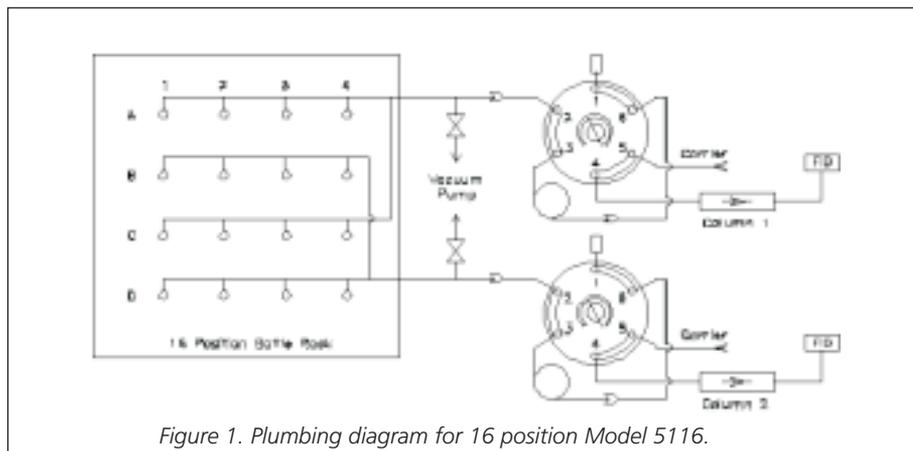


Figure 1. Plumbing diagram for 16 position Model 5116.

special report that can display the chromatogram for any bottle record. The locally customized database is then translated into the Series 5100. This translation sets up a spreadsheet that includes all of the required

information as defined by the database. This spreadsheet is saved in an Excel format. Using Excel®, the QC manager sets up a spreadsheet for each rack of bottles to be tested. This work can be done many days ahead.

Then, the technician collects the preforms based upon the directions of the spreadsheet. The bottles are then blown, purged with nitrogen and allowed to typically "soak" at temperature for 24 hours. The printed spreadsheet is usually left with the bottles. After bottles have soaked for 24 hours, the technician mounts the bottles in the test rack according to the locations specified by the spreadsheet. The bottles are automatically centered and held to protect the side-ported needles from bending. The electrical form of the same spreadsheet is then loaded into the Series 5100's main screen and the start button is pushed. When the test rack of bottles is completed, the spreadsheet is saved and then printed.

While each bottle is saved as an individual record in the database, the printed spreadsheet is an excellent summary for the QC manager.

## Why Save the Chromatogram?

The actual AA analysis is made using a gas chromatograph. A bottle's sample is injected into one channel of the chromatograph and is separated into its various components by a chromatographic column. The AA is eluted and measured by a flame ionization detector (FID). This detector output trace is called a chromatogram.

FID's are very sensitive for most carbon containing compounds. FID's also generate a peak in response to air. This air response is used by the system as a diagnostic.

To an auditor, an air peak means that the bottle was not sealed properly while it soaked for the day and the AA leaked out. If the AA chromatogram has no air peak, the analyst and the auditor can be sure that the bottle was purged with nitrogen and sealed. For this critical reason, the analysis chromatogram must be included in the bottle's database record.

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## PlaySafe Analyzer for Metals

### Helping to Ensure Child Safety

Headlines in the news continue to warn us about consumer products such as furniture, dishes, cosmetics, and most importantly, toys, contaminated with lead and other harmful metals. The U.S. Food and Drug Administration (FDA), U.S. Consumer Product Safety Commission (CPSC) and the European Union (EU), along with regulatory agencies in other countries are especially concerned about protecting the most sensitive population, children, from this threat

PerkinElmer has worked with manufacturers to develop the

PlaySafe™ Analyzer for metals, the first complete solution for this analysis. Based on the established inductively coupled plasma optical emission (ICP-OES) technology, to rapidly determine a wide range of metals in toys, the system includes everything the laboratory will need for rapid ramp-up.

### The PlaySafe Analyzer includes:

Optima™ 7300 DV ICP-OES instrument, rugged for laboratories in all parts of the globe and supported with service located in over 120 countries US or local controller Calibration standards Customizable

standard operating procedure (SOP) to provide step-by-step guidance on instrument operation associated with this method Instrument software method for the eight elements Specified in the EN-71, part 3 Application note showing the instrument performance Upon installation, users receive walk-through training on operating the method.



Example of the type of results obtained from the playSafe Analyzer (results in mg/kg in the original material before sample preparation).

	Antimony	Arsenic	Barium	Cadmium	Chromium	Lead	Mercury	Selenium
Yellow Plastic Car	600	14	104	<DL	3400	14800	6.0	<DL
NIST 1579a High Lead Paint	<DL	45	2.7%	20	200	11.8%	<DL	<DL
NIST 2582 Low Lead Paint	<DL	11	1860	<DL	30	205	6.0	<DL



EN 71-3, ASTM F963, 8 Toxic Metals