

# Fresh



HUMAN HEALTH | ENVIRONMENTAL HEALTH

VOLUME 9 | September 2009  
ANALYTICAL SCIENCES

Dear Readers,

It gives us immense pleasure to receive your valued comments and suggestions and patronage to the PerkinElmer for the products; solutions and services. In the previous editions we had tried to reach out to you with the technologies and new scientific innovations launched by PerkinElmer to suit various applications across the industrial and research segments.

In this issue we have focused on applications and solutions related to the Food & Beverages. The quality food for the mankind and its packaging to market are the key areas of many Food processing and export organizations. Along with that there are some simple knowledge inputs on the usage of the accessories for the instrument users are included here. Please go through the same and write to us for more information or suggestions.

Have a pleasant reading!

## FOR SAFER FOOD

WHAT'S  
**Fresh** inside...

- Clarus GCMS for the Analysis of Pesticides in Foodstuffs
- Analysis of Food-Packaging Film by Headspace - GC/MS
- Diffuse Reflectance Infrared Spectroscopy
- Analysis of Artificial Sweeteners by Diffuse Reflectance FTIR
- Packaging of Food & Pharmaceuticals ( A Blister Pack)
- LABWORKS food LIMS for the food industry



# The Application of GC/MS to the Analysis of Pesticides in Foodstuffs

William Goodman

PerkinElmer Life and Analytical Sciences 710 Bridgeport Avenue Shelton, CT 06484 USA

## Introduction

Pesticide contamination of foodstuffs has become a worldwide concern, prompting various levels of regulation and monitoring. Traditionally, pesticides are quantified with gas chromatography (GC) combined with selective detectors (ECD, FID, etc.).

Selective GC detectors are great tools to quantify one or two pesticide classes at a time. However, screening for a number of different pesticides requires multiple runs utilizing various GC configurations. Chromatographic run times are often long because of the need to achieve sufficient chromatographic resolution for unambiguous quantification. Gas chromatography / mass spectrometry (GC/MS) provides positive confirmation of various pesticides in a single analytical run; its superior selectivity allows interference-free quantification even with peak coelution. As a result, GC/MS has become a preferred technique for pesticide analysis because of its single-run capability.

This paper outlines a GC/MS method, allowing for the quantification of low-level pesticides with SIM, while simultaneously performing quantification of higher concentrations using full-scan acquisition (SIFI™- single ion and full ion scanning). It also demonstrates the throughput benefits of fast GC oven cool-down.

## Experimental

The PerkinElmer® Clarus® 600 GC/MS with programmable split/splitless injector was used for this application. The instrumental conditions used in this study are summarized in Table 1. Sample volumes of 1.0 µL were

injected into the programmable split/splitless injector, incorporating a 2-mm i.d. deactivated fused-silica liner.

The injection-port temperature was set at 275 °C (isothermal). The capillary column used incorporated a proprietary phase specifically suited for pesticides (Elite-CLPesticides) with the dimensions of 30 m x 0.25 mm x 0.25 µm df. The helium carrier gas was programmed with a constant velocity of 30 cm/sec. The oven-temperature program was initially set at 80°C with no hold and ramped to 290°C at 20°C/min with a hold of 4.5 minutes. The total oven program is 15 minutes, with an injection-to-injection time of less than 20 minutes.

Table 1. Instrument Conditions.			
Gas Chromatograph:	PerkinElmer Clarus 600 GC	Mass Spectrometer:	PerkinElmer Clarus 600 MS
Analytical Column:	Elite-CLPesticides (30 m x 0.25 mm x 0.25 µm)	GC Inlet Line Temperature:	275 °C
		Ion Source Temperature:	275 °C
Carrier Gas:	He (30 cm/sec)	Function Type:	SIFI
Injector Temperature:	275 °C	Scan Range:	m/z 40-450
Injection Type:	Splitless	Scan Time:	0.2 sec
Oven Program: Temperature	Hold Time	Rate	InterScan Delay:
80 °C	0 min	20 °C/min	0.1 sec
290 °C	4.75 min	end	



What's on my food.



The MS method contained multiple SIM functions overlapped by a  $m/z$  40 to  $m/z$  450 full-scan function. The timing and selected ions of each individual SIM function are dependent on the elution time and fragmentation of each pesticide of interest. The mass spectrometer transfer line and ion source were heated to 275 °C.

## Results and discussion

The maximum allowable level of pesticide residues in foodstuffs varies between countries. Japan, for example, has set a low level of 0.01 ppm. In this study, analytical standards comprised of organochlorine, organonitrogen and organophosphorous pesticides were analyzed between 0.01 ppm and 100 ppm.

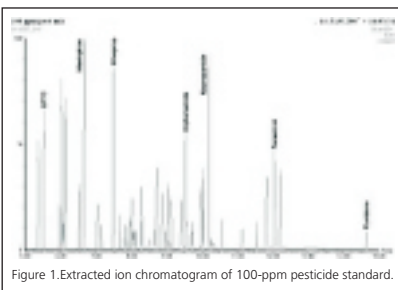


Figure 1. Extracted ion chromatogram of 100-ppm pesticide standard.

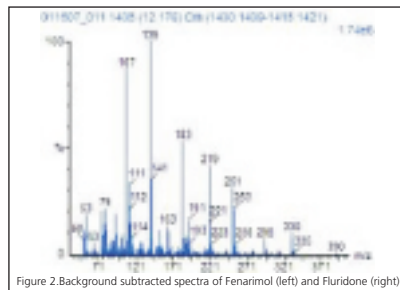


Figure 2. Background subtracted spectra of Fenarimol (left) and Fluridone (right).

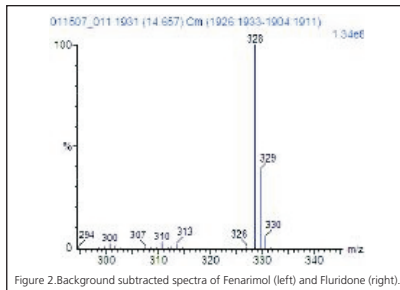


Figure 2. Background subtracted spectra of Fenarimol (left) and Fluridone (right).

The standards analyzed here contain over 50 pesticides, of which 25 are pictured in Figure 1. The chromatogram shown in Figure 1 is a composite of extracted ions from the full-scan acquisition of a 100-ppm standard.

The spectral data provided by the mass spectrometer allows for the use of chromatographic conditions that resolve only peaks with similar spectra, allowing for faster oven

programs and short analysis times. Pictured in Figure 2 are the background-subtracted spectra of Fenarimol and Fluridone. As you can see, the spectra of Fenarimol are quite complex and fragment into many different ions, while Fluridone is quite simple with only three major ions. When analyzing for pesticides with high levels of fragmentation, such as Fenarimol, achieving detection limits may become a challenge. The SIFI capabilities of the Clarus 600 MS will aid in overcoming these challenges. Additionally, SIFI will allow the acquisition of both full scan and SIM data simultaneously; the full-scan data will give library-searchable spectra, while SIM will allow for low-level quantitation.



# Analysis of Food-Packaging Film by Headspace-GC/MS

Miles Snow & Heidi Grecsek

PerkinElmer Life and Analytical Sciences, 710 Bridgeport Avenue, Shelton, CT 06484



## Introduction

Food-packaging material is typically manufactured as a thin film and coated with inks which usually contain multiple, harmful, volatile organics. Therefore, they must be carefully monitored and quantitated to ensure that the amounts are limited.

Traditionally, the test for solvent materials in food-packaging film was performed using a technique of heating a square meter of the film material inside a mason jar. This jar is then opened and tested (by smell) for volatile organic compounds. Later, this test was expanded to extract a headspace sample out of the mason jar by syringe and then injected into a gas chromatograph (GC) for quantitative analysis. This produced significantly better results and provided laboratories with a quantitative number. This process is still very time-

consuming and labor intensive as a result of the number of manual steps involved. The manual process of cutting food packaging, placing it in a mason jar, heating the jar, and manually collecting a sample for GC analysis dramatically limits the number of samples that can be analyzed each day. The technique demonstrated here will greatly improve the efficiency and throughput of this analysis.

This analysis can be completely automated using a PerkinElmer® TurboMatrix™ Headspace (HS) sampler with the Clarus®500 Gas Chromatograph/Mass Spectrometer (GC/MS) – see Figure 1. This system passed all the requirements for food-packaging analysis.

## Experimental

The first food packaging film used for this experiment was from a typical package of cookies. This film was cut into squares: 325 cm<sup>2</sup> pieces. The typical volume used in a mason jar is a square meter but this volume is not required for the headspace sampler. The desired sensitivity can be reached with significantly lower quantities. The second packaging material tested was obtained from a shopping bag that you would typically find at a department store. The 325 cm<sup>2</sup> pieces of film were added directly to a 22-mL

headspace vial. The vial was then sealed with silicone/PTFE septa (PerkinElmer part number B0104241). In addition, a calibration standard was prepared to get an estimate of the expected concentration of the typical solvents. This standard was prepared by adding 4.7 µg of each solvent in a 22-mL headspace vial (Table 2).

The instrument used for this analysis was a TurboMatrix HS 40 Headspace Trap sampler run in headspace-only mode. This bypassed the trapping capability. If extra sensitivity is required, the trap option could be used for up to 100 times lower detection levels. The shaker option on the headspace was utilized for a faster equilibration of the solid film material. The headspace was controlled using the TurboMatrix remote control software and was coupled to the Clarus 500 GC/MS. The Clarus 500 GC was equipped with a programmable split/splitless (PSS) injector and programmable pneumatic control (PPC). Deactivated fused silica (0.32 mm) transfer line connects the TurboMatrix HS 40 Trap to the Clarus GC.

## Results

The TurboMatrix HS 40 Headspace sampler was successful in analyzing the solvents in food packaging. Six solvents were identified: 1 – MIBK

(Methyl Isobutyl Ketone), 2 – NPAC (n-Propyl Acetate), 3 – ETAC (Ethyl Acetate), 4 – Propanol, 5 – ETOH (Ethanol) and 6 – Heptane (Figures 2 and 3). Ethanol and Propanol were the largest responders and overloaded the system. However, the requirements of the testing were to only get semi-quantitative information. Therefore, the overloading was accepted. All components were positively identified using a NIST library database.

The cookie package/wrapper had approximately 0.22 mg/m<sup>2</sup> of solvents found. However, Propanol was very significant, making up the large majority of the total solvents identified. The cookie wrapper also had a lower level of interferences from outside sources (Figure 2). The shopping bag (purple) had approximately 0.32 mg/m<sup>2</sup> of total solvent material (of the six solvents tested) – Table 2. This represented a very good response of all six solvents. In addition, there is a significant amount of other materials found in the food film. This is evident in the chromatogram shown on Figure 3. Because of the ability of the MS to extract only the required ion from the component of interest, this interference was not an issue.

The headspace system enabled the method to be set up and run unattended with no sample preparation. This eliminated the need for mason jars and operator attention. In addition, the system showed a significant amount of sensitivity for the required components, demonstrating the ease of setup methodologies of many types of food packaging at many different levels. The significant

response of the volatile solvent material by this heated headspace technique would allow for a flame ionization detector (FID) to be used as a substitute for the MS detector. While the MS gives a positive identification as well as selectivity, the FID can be used in a majority of standard QA/QC environments.



Figure 1. Clarus 500 GC/MS with TurboMatrix Headspace Trap.

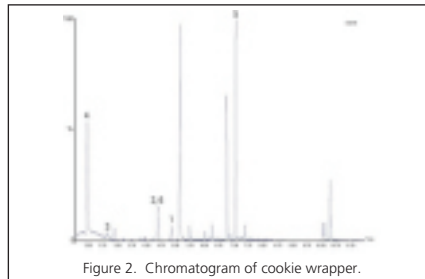


Figure 2. Chromatogram of cookie wrapper.

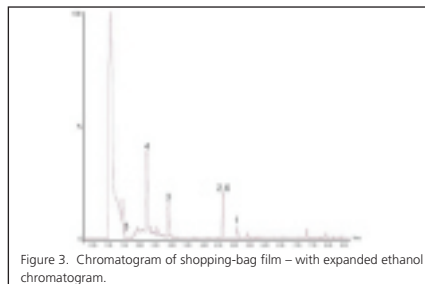


Figure 3. Chromatogram of shopping-bag film – with expanded ethanol chromatogram.



## Conclusions

The PerkinElmer TurboMatrix Headspace Trap with the Clarus 500 GC/MS meets all the requirements for food- packaging analysis. The main requirement for this application is fast, easy and quantitative solvent determination. Using the setup demonstrated here, the sample is placed into a vial and placed in the autosampler tray of the headspace. Then the automated analysis is completed without operator attention. In addition, the headspace's overlapping thermostating allows up to 12 samples to be processed simultaneously, thus allowing 50-75 analyses per day. For detail applications please log on to [www.perkinelmer.com](http://www.perkinelmer.com)

Table 2. Semi-Quantitative Results.

Sample: Standard					
Peak #	Solvent Name	RT (min)	Area	µg in Vial	
1	MIBK	5.104	15165890	4.7	
2	NPAC	4.663	19381950	4.7	
3	ETAC	2.932	14047220	4.7	
4	Propanol	2.256	16693610	4.7	
5	ETOH	1.518	31902978	4.7	
6	Heptane	4.69	12375010	4.7	

Sample: Purple Shopping Bag 300 cm<sup>2</sup>

Peak #	Solvent Name	RT (min)	Area	µg in Vial	mg/m <sup>2</sup>
1	MIBK	5.12	162823	0.05	0.00
2	NPAC	4.665	4010297	0.97	0.03
3	ETAC	2.927	4236236	1.42	0.04
4	Propanol	2.244	19894030	5.6	0.17
5	ETOH	1.526	15599010	2.3	0.07
6	Heptane	4.686	14941	0.01	0.00
<b>Total</b>				<b>0.32</b>	

Sample: Cookie Wrapper 325 cm<sup>2</sup>

Peak #	Solvent Name	RT (min)	Area	µg in Vial	mg/m <sup>2</sup>
1	MIBK	5.112	30410	0.01	0.00
2	NPAC	4.664	2320430	0.56	0.02
3	ETAC	2.947	472144	0.16	0.00
4	Propanol	2.243	21689300	6.11	0.19
5	ETOH	1.533	2630198	0.39	0.01
6	Heptane	4.692	211345	0.08	0.00
<b>Total</b>				<b>0.22</b>	

# An Introduction to Diffuse Reflectance Infrared Spectroscopy



Spectrum 100 FTIR with Plug-n-play DRA accessory

Diffuse reflectance spectroscopy in the infrared did not become a useful analytical measurement tool until late in the 1970's. It was the publication of the paper by Fuller and Griffiths (1) which led to the technique becoming an accepted means of obtaining spectra of powders. The optical design which they described was much simpler than previous designs, and when used with a rapid scanning FTIR yielded spectra which had significantly better and therefore, useful signal-to-noise levels. A typical commercial design is shown in

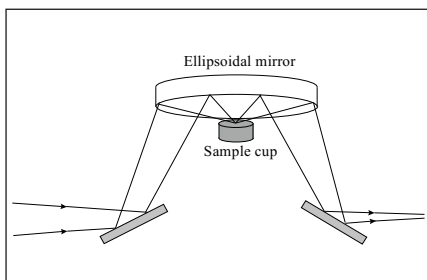


Figure 1. In general, designs of this type collect both diffusely (randomly) scattered radiation, as well as spectrally reflected radiation. It is only the diffusely scattered light that is of

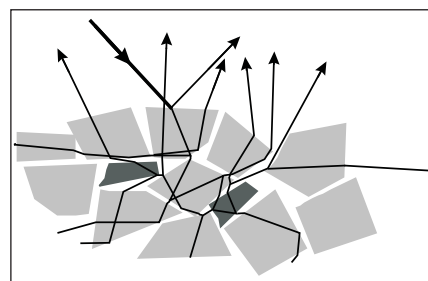
interest. Some designs provide for eliminating or substantially reducing the spectral component by tilting the sample holder, or by inserting a bar or post near the sample surface. The optical design of the accessories are described in detail elsewhere, i.e. in their instruction manuals, and will not be discussed further in this bulletin. Alignment of the accessory is critical, and this too is a subject of the instruction manuals.

The purpose of this bulletin is to briefly describe the theory of diffuse reflectance, to consider the limitations, and to present of art associated with the practice of using diffuse reflectance infrared spectroscopy. As part of this discussion, some consideration will be given to the proper operation of the FT spectrometer.

For infrared applications, the powdered sample is normally dispersed in a powder of an infrared transparent material such as KC1 or KBr. The orientation of the crystal faces of the sample and dispersing medium is random. Light is both transmitted through the particles and spectrally reflected from the surfaces depending on the angle at which the light strikes the surface. Higher angles of incidence (i.e. farther from the normal) leads to higher proportions of reflected light. The effect of the randomly oriented crystal faces is to randomly scatter the

incident light in all directions.

If a single incident ray is considered, then it will follow a random path through the nonabsorbent medium



either by weak surface reflection, or by transmission at the appropriate angle of refraction, until it comes to an absorbing particle, i.e. a small particle of the sample. If the angle of incidence into the sample particle is near to the normal, then most of the light is transmitted into the particle with only a small fraction being spectrally reflected. If, in addition, the frequency of the incident light corresponds to a vibrational absorption band of the sample, then the transmitted light is absorbed by the sample particle according to the normal laws of infrared absorption spectroscopy, that is, the Beer-Lambert Law  $A = abc$  -- where  $A$  is absorbance given by  $\log I_0/I$ ,  $a$  is the absorption coefficient for the vibrational absorption band,  $b$  is the particle thickness, and  $c$  is the concentration,  $I_0$  is the incident radiant power, and  $I$  is the transmitted radiant power.

If the angle of incidence at the sample particle is large more of the light is reflected. Reflection in the vicinity of bands with high absorption coefficients exhibits anomalous behavior resulting from the refractive index change across the absorption bands, making the band shapes asymmetrical.

The resulting spectrum will contain contributions from both absorption and reflection. There are several limiting cases which will make the appearance of the spectrum more understandable.

1. Small particle size, low absorption coefficient, low concentration. The product of these is equal to absorbance, as noted previously. The implication of all of these factors being small is that not all of the light incident light is absorbed, and that a finite amount is scattered back through the surface and measured by the instrument. If the absorption coefficient is small, then the anomalous surface reflectance will also be small and most of the scattered light will contain information about the absorption characteristics of the sample. If the particle size is small, such that total absorption does not occur, then once again the resultant measured intensities will be more typical of the absorption than of the reflection. In the near Infrared where the absorption coefficient is smaller by one to several orders of magnitude than in the mid-infrared, diffuse reflectance spectra have been shown to be very useful for quantitative measurements. In the mid-infrared, concentrations in the several percent range have typically been used with the result that the spectra tend to be significantly distorted by the surface reflection and subsequently, to be less useful quantitatively.
2. Large particles, high absorption coefficient, high concentration. The fact that each of these factors is large means that most of the light will be absorbed, and the

resultant scattered light will be more related to the magnitude of the reflected light from the crystal surfaces. It should be noted that the reflection will be determined by the refractive index and will, therefore, have an anomalous appearance across an absorption band.

3. A distribution of particle sizes, moderate absorption coefficient, moderate to low concentration. This case should be closer to the general real-life case. Some strong bands will be distorted significantly, while the weaker bands will be more useful for quantitation. Qualitatively, the spectra will be useful for identification, but the relative band intensities will not be the same as measured by transmission using the KBr disc or mulling technique.

#### SAMPLE PREPARATION

For mid-infrared measurements it is important that the particle size not exceed a thickness where total absorption would occur. For polar compounds this means thickness of 25  $\mu\text{m}$  to 100  $\mu\text{m}$  for most absorption bands. Transmission techniques such as the KBr disc or mulling technique require particle sizes less than the wavelength by about one order of magnitude i.e. 1 to 2  $\mu\text{m}$ . This is a much more severe requirement than for diffuse reflectance, requiring more severe grinding with greater possibilities for polymorphic changes or chemical modifications.

Following the moderate grinding step, the sample is mixed with a non-absorbing medium such as KBr or KC1 powder. This is also a gentle step resulting in less water absorption on the KBr or KC1 surfaces than for transmission methods. The concentration should be small for the mid infrared, generally less than 1% by weight in the non-absorbing medium. Mixing of the sample with KBr should be done in such a way as to maximize uniform distribution. This may be done

by mixing in several steps. The ground sample can be placed in a mortar and a roughly equal volume of KBr added and mixed. Subsequent additions of KBr should roughly double the volume each time until sufficient KBr has been added to fill the sample cup.

The mixture is then placed in the sample cup and the surface wither lightly compacted to make it flat, or scraped with a spatula held at about 45 degree angle. The idea is to produce a diffusely scattering surface, not a spectrally reflecting one.

#### INSTRUMENT OPERATION

Generally some 5 to 15% of the incident radiation will be scattered into the instruments optical path to be measured. While this is a small amount of light to recover, it is quite sufficient to allow good analytical measurements to be made with a Fourier Transform instrument fitted with a DTGS detector. If an MCT detector is used, it may be necessary to reduce the amount of light reaching the detector by additional aperturing of the beam, or by introducing an attention via a screen in order to prevent saturation and non linear detector effects.

Since most condensed phase absorption bands have half widths of 4 to 8  $\text{cm}^{-1}$ , the instrument resolution should be set to be about these values. A sufficient number of scans should be averaged to yield the desired signal-to-noise; typically this should be one to two minutes of data acquisition time. Of course, these values for resolution and time will be adjusted to fit the specific sample and questions being asked about the sample.

#### KUBELKA-MUNK FORMAT

If the absorbance is small, it is not strictly necessary to go to the Kubelka-Munk format for quantitative determinations. If the absorbance is moderate, then the Kubelka-Munk format should be used.

# Analysis of Artificial Sweeteners by Diffuse Reflectance



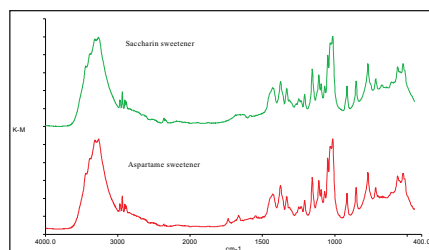
Reading labels on off-the-shelf products is generally quite revealing. For example, the first component, which is normally the highest concentration component, listed on the labels of the two most common artificial sweeteners is dextrose. The actual sweetener content is often in the low percentage level. Infrared spectra of these materials is easily obtained by diffuse reflectance since products like artificial sweeteners occur as finely divided powders which require no further grinding and only have to be mixed with KBr powder to prepare the sample for diffuse reflectance. It is the purpose of this bulletin to compare the spectra of a saccharin based sweetener with a phenylalanine based sweetener.

## Experimental

All spectra were obtained using a diffuse reflectance accessory in a PerkinElmer Paragon Fourier Transform Spectrometer. A background spectrum was obtained by placing infrared quality KBr powder in the diffuse reflectance cup and packing it lightly to obtain a flat diffusely reflecting surface. Some 256 interferograms at 4cm<sup>-1</sup> resolution were averaged for the background. Weak apodization was applied.

Samples were prepared by mixing about 5mg of sample in 300mg of KBr. In order to insure a homogeneous mixture, the weighed 5mg sample was placed in a mortar

## Results and Discussion



and ground lightly and mixed with an equal volume of KBr. Aliquots of the KBr powder were added doubling the volume in the mortar with mixing between each addition until all of the 300mg of KBr had been mixed. The mixture was transferred to the clean diffuse reflectance sample cup, packed lightly and levelled. Some 64 interferograms were averaged and ratioed against the stored background. Spectra of the saccharin based and phenylalanine based sweeteners are shown in figure 1. It can easily be seen that the two spectra are very similar with exceptions occurring near 1700 and an inversion in relative intensities of the two weak bands near 1250cm<sup>-1</sup>. In the 1650 region the saccharin based material shows a broad weak band while the phenylalanine based sweetener has a pair of sharp bands at 1736 and 1664cm<sup>-1</sup>.

Those bands which are common to the two spectra may be assigned to dextrose. As noted previously, dextrose is the highest concentration component in both sweeteners and it

should be expected to dominate the infrared spectrum. Table 1 summarises the contents of the two sweeteners.

### Sweetener 1

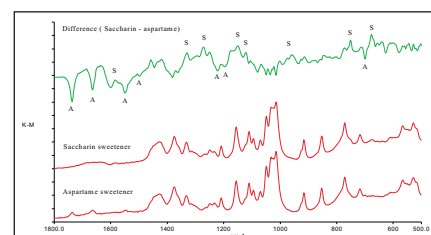
- Dextrose
- Maltodextrose
- Aspartame (l-aspartyl-l-phenylalanine methyl ester)

### Sweetener 2

- Dextrose
- Calcium saccharin cream of tartar (mono-potassium tartrate) calcium silicate

It is difficult to assign any of the minor bands directly except those at 1736 and 1664cm<sup>-1</sup> which come from the aspartame. However the bands due to dextrose can be largely eliminated by subtracting one spectrum from the other with appropriate scaling. In the difference spectrum a number of the major bands from the saccharin and aspartame components can be recognised from reference data. These are indicated with S and A respectively in the Figure below.

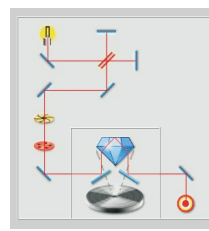
A better procedure would be to generate a spectrum of dextrose and subtract this directly from the spectra of the individual sweeteners.



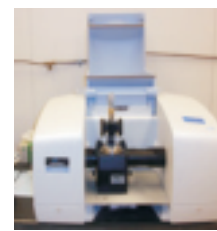
# Packaging of Food & Pharmaceuticals (A Blister Pack)



Typical Blister pack tablets



The light path for Universal ATR accessory



PerkinElmer Spectrum 100 FTIR with ATR accessory.

Many over-the-counter non-prescription pharmaceuticals & food items are packaged in what is called a blister pack. The structure may be a paper label with some printing on the back of the pack. This is bonded to an aluminum foil which in turn is coated. The tablet or capsule lies on top of this coating and a clear polymer is sealed over the top with a "blister" in it which encloses the tablet or capsule. In order to understand the cost of this structure it is necessary to know the identity of the components as well as their weights (or thickness). The latter can be determined by weighing a defined area and will not be discussed further.

## Experimental

All infrared spectra were obtained using a PerkinElmer Fourier transform spectrometer and a horizontal internal reflection accessory fitted with a ZnSe crystal. Spectra were measured at 4cm<sup>-1</sup> resolution using weak apodization. In all cases the spectra are 4 sample scans against 16 background scans.

Pieces of the blister pack were cut to obtain flat portions which were used singly or in several pieces to obtain a large enough area to fill at least the height of the internal reflection crystal and some lateral distance. Pressure was applied to the sample/crystal interface in order to improve optical contact and therefore, useable intensities in the spectra.

## Discussion

Spectra were obtained from the paper

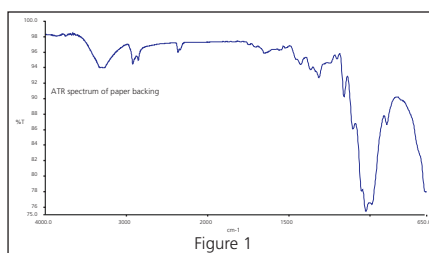


Figure 1

backing, from both sides of the clear polymer cover, and from the coated aluminum foil under the tablet. The adhesive between the paper and the aluminum foil was not examined.

Figure 1 is the spectrum of the paper backing. This is the spectrum of cellulose and it may be concluded from this that the paper is not coated. Spectra from the two surfaces of the

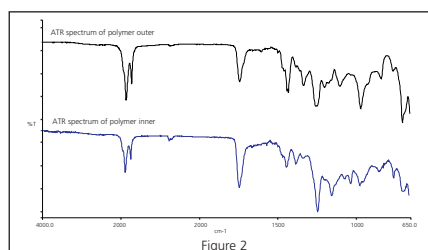


Figure 2

polymer cover are shown below. The outside consists of a vinyl chloride/vinyl acetate copolymer with a ratio of about 97/3 for the two monomers. The inside is also vinyl chloride/vinyl acetate but with a monomer ratio of about 85/15. Comparison with reference spectra indicates there is at least one other component contributing to this spectrum. Examination of the spectrum of the coating on the aluminum, Figure 3, revealed the probable source of this additional component. Figure 3 is the

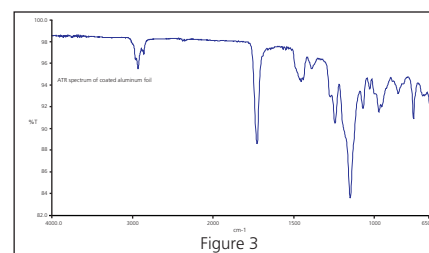


Figure 3

spectrum of an acrylate which was tentatively identified as poly-n-butyl methacrylate. The strong band near 1142 cm<sup>-1</sup> in this spectrum is also easily seen in the lower spectrum of Figure 2. In addition, the sharp band near 748 cm<sup>-1</sup>, the weak band near 1062 cm<sup>-1</sup> and the broadening of the carbonyl band on the low wavenumber side and the band near 1440 cm<sup>-1</sup> are supportive of the suggested source of the additional component in Figure 2 being some transfer from the coating on the aluminum.

It is possible that there is another component in the clear cover which lies between the top and bottom layers and assured their bonding together. Infrared microscope studies of thin edge sections of the cover are suggested as an approach to resolve this question. Transmission measurements were attempted but the film was too thick to obtain useable spectra. It must be emphasized that the appearance of different polymers on the two sides of the clear cover should serve as a warning to examine all surfaces by internal reflection or other techniques in order to avoid drawing erroneous conclusions.

# LABWORKS foodLIMS™



Meeting regulatory requirements and competitive pressures

Companies producing food and beverages are undergoing tighter regulations and increased scrutiny from government agencies and consumers at the same time that competitive pressures are increasing.

The Bioterrorism Act of 2002 mandates that food and beverage producers be able to accurately trace their products both backward into the supply chain and forward through the distribution system.

Food and beverage producers face the challenge of meeting safety and increasing tighter quality standards while reducing costs to meet the challenges of global competition.

Manual entry of chemical analysis data is labor intensive and creates the potential for typographical errors.

Manual data entry for chemical

analyses creates a time lag between laboratory analysis and approval and the availability of data in operational systems.

## Approach

The Laboratory Information Management System (LIMS) and implement interfaces with laboratory instruments, such as PerkinElmer's Series 200 and 275 high performance liquid chromatography (HPLC), Lambda™ UV/Vis, Clarus® series gas chromatography (GC) and inductively coupled plasma mass spectroscopy (ICP-MS). Also implement interfaces with food safety software, quality analysis software and operational software.

## Recommendations

Select PerkinElmer LABWORKS to replace legacy laboratory data

management systems and increase your organization's productivity and data quality.

- Assess the current data systems capability in terms of connectivity, productivity and quality. Assess the benefits and ROI associated with an upgrade to LABWORKS
- Partner with PerkinElmer LABWORKS. With over 20 years of experience providing successful LIMS implementations, LABWORKS has well established partnerships with leading food industry, quality analysis and operational information systems as well as project management/project implementation solutions providers
- Implement systems integration to link your laboratory data with your raw material acceptance and product release processes to effectively increase organizational productivity and data quality.

## Partner with LABWORKS to increase productivity and secure compliance today and in the future.

### Results

- LIMS technology reduces record keeping and eliminates most of the paperwork that analysts currently have to perform:
  - The software automatically generates labels for each of the tests required for every batch of raw and intermediate material and finished product
  - Analysts can simply scan the label to enter all of the information required about the test
  - As soon as the test is completed, the test results move into the inbox of the person that is responsible for the first level of approval
  - As each level of approval is completed, the results automatically move to the next level approver
- In a typical application at a food and beverage company, analysts were able to perform 50% more tests, streamlining operations:
  - The integration of the LIMS with existing customer software that enable backwards and forward tracing of the supply chain helps with compliance to the Bioterrorism Act of 2002 and other regulatory requirements
  - Automated workflow dramatically reduces the time required for a work order to proceed through the system
  - Automatic data entry and movement greatly reduces the potential for data entry and transcription errors
  - Internal customers can now view the data as soon as it is collected and validated. They can log in at any time to determine the status of a work order or view the results of tests that have been completed
  - External customers can also be granted access to test results and status information
  - The interface between the laboratory instruments and the LIMS saves time and improves accuracy by automating the process of transferring results from the various instruments to the LIMS
- LABWORKS integrates with SAP® R/3® (and other ERP/MRP applications) to capture the tests that are required for current production so that samples can automatically be logged in. When the tests are completed, the SAP® interface automatically sends the results back to SAP® for easy access by manufacturing and can also automatically distribute them. The SAP® Interface also automatically keeps track of product shipments and generates a certificate of analysis with the exact information required by each customer
- LABWORKS integrates with PathTracer® to link test results to the inbound ingredients through processing by lot code including packaging to a specific batch of the finished product. This approach limits liability risk by helping to manage the recall to only the specific batches that need to be recalled.
- LABWORKS integrates with Northwest Analytical's Quality Analyst® to enable users to graphically analyze process behavior and judge the impact of process improvement decisions with minimal training in statistical techniques.

### Partner Solutions

LABWORKS™ provides software and services to effectively bridge the gap between the laboratory and operations. Partnerships with key industry applications take management of laboratory data to a new level.