TOP 100 of 2002 chosen
GERSTEL among the most innovative medium-sized companies in Germany

Berlin/Mülheim an der Ruhr, Germany – The one hundred most innovative medium-sized companies in Germany for 2002 have been selected – GERSTEL GmbH & Co. KG from Mülheim an der Ruhr is among this „TOP 100“. The expert panel of the „Best of TOP 100 Germany Innovation Competition“, under the patronage of Dr. Hans-Jürgen Warnecke, president of the respected German Fraunhofer-Gesellschaft in Munich, came to this conclusion.

This is the eighth time the competition has been held. It promotes the performance of the companies chosen and the image of medium-sized companies, the „backbone of German business“ according to Warnecke. „In Germany there are around 30,000 medium-sized companies that undertake research and development“, said Warnecke at the prize ceremony in Berlin. A significant number, considering many medium-sized companies are contractors. Because these companies aren’t in the news like large companies are, it is easy to overlook the fact that they are the real motor of the economy.

Innovative medium-sized companies are distinguished, said Prof. Dr. Hans Hörschgen, Professor of Economics at the University of Hohenheim, in which details of each company, such as its economic development, its innovation in the areas of product, organisation, personnel and company culture, were evaluated. „Companies were selected if they demonstrated success in these areas as measured by increased competitiveness – and GERSTEL fulfilled the qualification“, said Holger Gerstel, managing director and co-owner of the Mülheim company.
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Editorial

Overwhelming Customer Response

When you visit any of the major science trade shows, it is clear that all companies focus considerable effort on obtaining complete customer satisfaction. Achieving this requires continuous improvement in all services provided to the customer and not taking even the smallest detail for granted.

GERSTEL sees itself as your partner. We have made it our mission to provide you with the tools needed to solve your most difficult analytical problems, and we want to continue to develop and customise these tools to suit your individual needs. In order to do this, we collaborate closely with our customers, because we can’t provide useful solutions unless we fully understand your needs.

The overwhelming response that we received this year at the trade shows we participated in, show that our customers agree with our approach. Never in the history of our company have we experienced such response to our products and complete analytical solutions.

It was also very heartening that many of the people that came to our booth were excited about using our new products to solve their existing analytical problems. This is further proof that we are reaching you and that we are on the right track.

Many thanks for the great trust that you have placed in us. I hope that we will continue to benefit from our successful partnership and that you will enjoy the articles in this special trade show edition of GERSTEL Solutions worldwide.

Yours sincerely

Holger Gerstel
Managing Director
GERSTEL GmbH & Co. KG

Impressions of Analytica 2002

Trade fair review 2002

Precision landing for new GERSTEL products

...Despite careful attention to customer needs during product development, we are never really sure in advance how clients will react to a new product introduction. Once a new product is launched at a trade fair, we get a clearer picture of the impact of new products." After numerous technical developments and trade fair visits, Ralf Bremer, Technical Director of GERSTEL GmbH & Co. KG, knows what he is talking about. This year, the company has already presented its new products several times to a wide professional public at important scientific expositions, including the PittCon Conference in New Orleans, USA; Analytica in Munich, Germany; and the 25th International Symposium on Capillary Chromatography in Riva del Garda, Italy.

Bremer believes that the results so far confirm this: "We have achieved successful launch and precision landing with our new products and customer-oriented solutions."

Applications-oriented work was the focus of PittCon in March of this year. "Our company presented ten technical posters with applications", says the manager, "more than ever before." Among these posters were applications of the new GERSTEL Headspace ChemSensor.

At Analytica, the main focus was automatic thermal desorption using GERSTEL Twisters by means of the new Twister Desorption Unit TDU and Multi Purpose Sampler MPS_Twister Option. Designed specifically for Twister desorption, the TDU unit can be used with the MPS Twister Option to automatically process 196 Twisters. "The great interest in the TDU suggests that Twister Star Bar Sorptive Extraction (SBSE) will increasingly become the sample preparation and extraction technique of choice", says Bremer.

Many visitors to the exhibit at Analytica, with 30% higher attendance than 2000, were interested in new developments with the GERSTEL Multi Purpose Sampler MPS 2, including the new PrepStation with SamplePrep software. The PrepStation is the latest MPS 2 system, providing full automation of both sample preparation and sample introduction steps for higher analytical productivity.

The PrepStation is a unique dual-rail, dual-robot configuration of the MPS 2. Bremer asserts that the most distinctive feature of the PrepStation is its control software, which enables very complex processes to be performed extremely simply - "without any need for macro programming", Bremer emphasized. The PrepStation was also a big hit at PittCon.

GERSTEL presented eight scientific publications at Riva. Among these were papers describing use of the new Headspace ChemSensor in applications such as classification and quality measurement of constituents in food and beverages. Lectures presented by GERSTEL scientists attracted a great deal of attention, said Bremer, with audiences of at least 150 people.

"It is striking", says the manager, summarizing his impressions, "that more and more users are seeking effective, economical solutions that can be tailored to their individual needs. These needs are satisfied with the flexibility of the GERSTEL Modular Analytical Systems concept, which provides for customer-specific modifications."

New product: TDU

When combined with an MPS 2, allows automatic processing of up to 196 Twisters with the GERSTEL Thermo Desorption Unit TDU.

November 02
Het Instrument
Utrecht, Netherlands
04. – 08.11.2002
Pollutec
Lyon, France
26. – 29.11.2002
expoquima
Barcelona, Spain
26. – 30.11.2002
March 03
Pittcon 2003
Orlando, Florida, USA
09. – 14.03.2003
Further information on dates, exhibitions and products on the internet at www.gerstel.de.
Membrane Extraction versus Liquid-Liquid Extraction

Effluent analysis made easy

Membrane-supported solvent extraction

For membrane extraction, 8 to 10 membrane bags were conditioned by soaking three times with 50 mL hexane at room temperature. The vial was filled with 15 mL aqueous sample, the membrane bag was fixed to the sample vial using a Viton ring, and the funnel was suspended in the opening of the vial. Finally, the membrane bag was filled with 500 µL hexane to which 1 mL of the simetryne internal standard was added, and the vial was sealed with a metallic crimp cap.

For extraction, the vial was placed in the interval shaker of the MPS and shaken for a defined time at a set temperature. Finally, it was automatically removed from the MPS and transferred to the sample vial. The organic extract was removed manually from the membrane bag using a microlitre syringe and transferred into a 2 mL sampler vial.

Editor’s remark: In the time since this study was performed a new PrepStation software for the Multi Purpose Samplers MPS has been released. This software allows automation of all steps of the Membrane Extraction method.

LLE of river water

In order to compare the quantitative results of membrane-supported LLE with in-vial LLE without a membrane, 15 mL river water was filled in a 20 mL headspace vial with 1 and 5 µL of each analyte and 1.3 µL pentachlorobenzene as internal standard. After introduction of 1 mL hexane, the vial was sealed with a metal crimp cap and shaken for 30 minutes at 35 °C at a rate of 750 rpm in the MPS-2 interval shaker. The organic extract was removed using a microlitre syringe and transferred to a auto sampler vial. Large Volume Injection was used for GC/MS analysis with an injection volume of 100 µL. Direct calibration of the LVI/GC-MS was achieved with mixed standards in hexane and an injection volume of 100 µL (1 µL/s) for determination of the analytes spiked in river water.

Results and discussion

Membrane-supported solvent extraction

With Membrane Extraction, hydrophobic organic compounds are extracted through a membrane into a small volume of organic solvent. Relatively non-polar solvents are used, since they have low solubility in water, and solvent loss through the membrane is avoided. On the other hand, very polar solvents can be used with minimal loss through the membrane. Water-miscible polar solvents cannot be used for normal LLE. This is different for Membrane Extraction, because they do not get in contact with water phase. In a pilot HPLC study, polyaromatic hydrocarbons were successfully extracted from aqueous samples using acetonitrile inside the membrane bag.

The solvent should also be too volatile, since it may diffuse through the membrane and into the headspace of the sample and condense there. It needs to be volatile enough, however, to be removed effectively by the split vent during the LVI.

Editor’s remark: GERSTEL supplies ready-prepared membrane bags with a wall thickness of 0.03 mm, suitable for the application described here, and tested with cyclohexane as the solvent.

Optimisation of the extraction parameters

Effect of matrix constituents

Table 1 (page 6) shows the optimised parameters affecting membrane-supported solvent extraction: salt, methanol content and pH. If the solution is saturated with NaCl, extraction of triazines is improved; these are relatively polar analytes. By contrast, the recovery rate of the non-polar constituents α-HCH and pentaeranthene slightly fell if the methanol content was increased to 6.66 Vol%. It had no significant effect on the extraction of most constituents, with exception of S-triazines, whose recovery rate fell to 10 to 20 %.

The pK values of the aqueous sample should therefore by somewhat higher than 6; an even higher pH value does not improve the extraction results. For all extractions, the aqueous samples were saturated with 333 g/L NaCl (5 g NaCl in 15 mL water).

Optimisation of shaking rate

The sample must be mixed thoroughly and the boundary layers in the membrane bag minimised, in order to improve the transport of the analytes through the membrane into the organic solvent. The shaking rate of the MPS 2 was varied between 250 and 750 rpm. The extraction yields increased for all analytes by 30 – 50 % when agitation speed was increased to 500 rpm; further increases in speed gave only minimal increased yield. Mixing is more important for triazines than for the non-polar constituents α-HCH and pentaeranthene; for all further studies, the shaking rate of the MPS 2 was therefore set at 750 rpm.
Optimisation of temperature

The interval shaker of the MPS 2 can be set to a defined temperature. Increasing the temperature during the shaking phase from 35 to 55 °C (hexane boils at 69 °C) improved the recovery of all constituents by 10 to 30%; the effect was particularly marked for water-soluble triazines, and less for 2,4-dichloroaniline, each component. 100 µL injection (b): extraction duration 1 h, 333 g/L NaCl, 45 °C, 750 rpm.河

Optimisation of extraction time

An extraction time of 30 minutes led to optimal recovery of all components (Figure 2); increasing the time did not lead to any improvement. After 30 minutes, the recovery was 60 to 100 %, sufficient for validation of the method.

Valuation of method

The performance of membrane-supported solvent extraction was tested under optimised extraction conditions; table 2 shows the validation results. The linear dynamic range was determined by extraction of spiked aqueous samples, and for 10 µL ranging from 0.05 to 100 µg/L; the regression coefficient was 0.9965 or better. After 30 minutes extraction, the detection limit of 10 to 100 ng/L, was achieved (see summary).

The detection limits were determined by blank values, extraction was carried out at 55 °C for subsequent 10-µL injection.

The analytical accuracy of in-vial extraction was better than that of membrane-supported solvent extraction (Table 3). The mean variation of analytical results from the spiked concentration values was: 12.4 % for in-vial LLE with 5 µg/L spiked river water and 22.9 % for Membrane Extraction, which is, however, easier to perform: if an injection volume of 100 µL was used, the whole procedure, that is extraction and injection, can be fully automated.

Summary

The Multi Purpose Sampler MPS 2 allows complete automation of membrane-supported solvent extraction, which is a promising enrichment technique for various organic and inorganic compounds, besides polar analytes such as triazines: under optimised conditions with an extraction time of 30 minutes, recoveries of 60 to 100 % were obtained. The detection limits were in the low ng/L range. After the non-porous polypropylene membrane back washes the protein, water-soluble matrix components in the blanks originate from the heat-sealed bag made of polypropylene. Membrane Extraction is especially suitable for complex samples with a high organic content.

Membrane Extraction is especially suitable for applications in food analysis and bioanalysis: by choosing solvents that are miscible with water, such as acetonitrile, the method can be used with reversed phase HPLC. Polar solvents do not dissolve in the membrane material and therefore cannot pass into the aqueous sample.

In combination with GERSTEL MASTIS software, in sample preparation mode, the MPS 2 allows automation of a sequence of membrane-supported solvent extractions, giving high sample throughput.

Conclusion

GERSTEL Membrane Extraction, shown here with the example of triazines and other semi-volatile contaminants, with direct coupling to Large Volume Injection and GC-MS detection is an advantageous procedure in terms of cost and time for investigation of effluent and brackish water with high content of suspended material. It fulfills the requirements of the German Drinking Water Ordinance (0.1 µg/L for individual pesticides) [2] and Drinking Water Recommendations of the World Health Organisation WHO [2] (µg/L atrazine and simazine) [3].

Literature

(2) TVO-BRD, appendix 24, 01.04.1998.

Figure 3: UHPLC-Chromatogram of Single-Ion Monitoring after Membrane Extraction of 15 mL water, spiked with 0.5 µg/L each component (extraction time 1h, 333 g/L NaCl, 45 °C, 750 rpm, injection volume 100 µL)

**Table 1**

<table>
<thead>
<tr>
<th>Component</th>
<th>Extraction yield [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extracted water</td>
<td>8.2 µg/L NaCl</td>
</tr>
<tr>
<td>Recovery</td>
<td>95.0</td>
</tr>
</tbody>
</table>

**Figure 2**

Enrichment of all components; increasing the time did not lead to any improvement. After 30 minutes, the recovery was 60 to 100 %, sufficient for validation of the method.

**Table 2**

<table>
<thead>
<tr>
<th>Component</th>
<th>Recovery [%]</th>
<th>Detection limit (µg/L)</th>
<th>Linear dynamic range (µg/L)</th>
<th>Accuracy of peak integration at low concentrations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extraction</td>
<td>60 to 100 %</td>
<td>0.001 – 100</td>
<td>0.9965 or better</td>
<td>Co-extracting matrix components; components in the blanks originate from the heat-sealed bag made of polypropylene.</td>
</tr>
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<td>Membrane Extraction</td>
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<th>Component</th>
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Pesticide residue analysis is usually costly and time-consuming. Analysis of individual pesticides or classes of pesticides e.g. organochlorine pesticides (OCPs), organophosphorus pesticides (OPPs), triazines, etc., is more and more replaced by multiplex methods. The first aim of a multiplex method (MRM) is to detect as many pesticides as possible with one analytical technique including sample preparation and chromatographic analysis. Only after elucidation of the pesticides in a specific matrix, accurate and precise quantification can be performed. In recent years important improvements have been made in multiplex analysis by capillary gas chromatography – mass spectrometry. Through the features of Electronic Pneumatic Control (EPC), Retention time Locked Libraries (RTL) for GC amenable pesticides and endocrine disruptors could be constructed and by linking the locked retention times to the mass spectral data hardly any pesticide that is in the library can escape detection and elucidation [1, 2]. The Agilent Technologies RTL-MS library presently comprises 567 substances. A versatile sample preparation technique for the enrichment of pesticides from different matrices and came to the conclusion that 440 pesticides out of the RTL-MS library can be enriched from water, beverages, fruits and vegetables, with recoveries complying with the required Limits Of Quantification (LOQ) set by regulatory organizations. The complete list of pesticides amenable to Twister enrichment and RTL-Capillary-GC-MS analysis will be published in one of the next issues of LC-GC Europe [3]. The recent introduction by GERSTEL of the new Twister Desorption Unit TDU that can be installed on the MPS 2 enables fully automated analysis of 98 or 196 Twister stir bars. This makes the application of this new MRM very cost-effective. The principle and potential of Twister-RTL-Capillary-MS is illustrated with the determination of pesticides in grapes. The sample preparation, valid for all fruits and vegetables, is as follows: 1.5 gram grapes purchased from a local supermarket were mixed with 30 mL methanol and 1 mL of the extract was diluted with 10 mL water. A Twister was added and stirred for 60 min. The Twister was then desorbed at 280 °C (5 min) in the splitless mode at 50 mL/min and the solutes were cryofocused at –100 °C. The GERSTEL CIS operated in the splitless mode was then programmed at 600 °C/min to 280 °C (2 min). Analysis was done on an Agilent Technologies 6890 GC with 5973 MSD combination equipped with a 30 m x 0.25 mm I.D., 0.25 µm HP-5MS column. The oven temperature was programmed from 70 °C - 2 min - 25 °C/min - 150 °C - 3 °C/min - 200 °C - 8 °C/min - 300 °C. This is the RTL program and locking was performed on p,p’-DDT (26.999 min). The MS was operated in the scan mode (m/z 40-500). Figure 1 shows the total ion chromatogram and on this chromatogram the RTL screen was applied. Figure 2 shows a typical screening result. Perme-thrin II is identified through its retention time and four specific ions. The total screening then gives all pesticides positively identified in the grapes (Figure 3) and by standard addition the quantities could be measured. Note that chlorpyrifos is present at the 0.1 ppb level which means that whatever the matrix is e.g. drinking water, beverages, fruits, vegetables, etc., limits of determination can easily be reached in the MS scan mode.

Acknowledgement

My coworkers and co-authors of the article in LC-GC Europe, F. David (RIC) and B. Tienpont (Ghent University) are thanked for their contribution.

References


Figure 1 Total ion chromatogram of Twister-RTL-Capillary GC-MS of grapes

Figure 2 Total ion chromatogram of Twister-RTL-Capillary GC-MS of grapes
The GERSTEL Thermal Desorption Unit (TDU) is a designed instrument for use with GERSTEL Twister stir bars. The TDU is used in combination with GERSTEL’s Cooled Injection System (CIS) on a GC or GC/MS system to enable ultra-trace analysis of aqueous and other liquid samples.
Further international expansion

GERSTEL is continuing to expand steadily and is now represented in 40 different countries. Most of the company’s approximately 100 employees around the world are located in Germany - at the headquarters in Mülheim an der Ruhr and at the production facility in Duisburg. The company does, however, also have a US subsidiary, GERSTEL Inc., which is responsible for North America (the biggest market in the world for instrumental analysis), Mexico and Canada, and GERSTEL AG in Switzerland. In 33 countries GERSTEL is represented by distributors (see page 10 and 11). In the past three years, GERSTEL succeeded in establishing itself and performing effectively on the growing Asian market in particular. The company is now focussing its operations primarily on Eastern Europe as well; contracts have been concluded with distributors found in Russia, Belarus, Ukraine, Mongolia and Hungary. Eastern Europe is considered to be a very promising overall market with tremendous growth potential.

Visualisation of olfactory intensities

When analysing aromatic substances, conventional methods rapidly become inadequate. Only when sensitive analytical tools and the human senses, in this case the nose, are used in parallel, can meaningful and reliable information be obtained.

The GERSTEL Olfactory Detection Port (ODP) 2 adds an „aromagram“ of the sample to the chromatogram, for detection of either a single substance or a complex pattern of aromas. The ODP 2 allows (by combination of a commercial gas chromatography with mass-selective detection) clear-cut characterisation of aromatic compounds.

The development of the new GERSTEL Olfactory Recording Software package makes a significant contribution to olfactory analysis. Now the aromagram can provide 4 levels of aroma intensity and be annotated with text that is produced during the olfactory analysis. This is how it works. When an aroma is detected, one of four keys is pressed on a USB based Olfactory Intensity Pad. The four keys provide four intensity levels that are represented as different peak heights in the aromagram. The aromagram is then stored with data from any other detectors connected in parallel with the ODP 2. Pressing a key also activates the voice recording function and the aroma description spoken during that time is also stored along with the aromagram.

Once the olfactory analysis is completed, the spoken commentary can be reviewed, and corrected if necessary. A complete report can be generated that contains aroma detection times, descriptions and GC run information.

MAster Software now integrated in GC-ChemStation from Agilent Technologies

Simple, rapid and comfortable

In the past, if you wanted to use the GERSTEL Thermal Desorption System (TDS) or the GERSTEL Cooled Injection System (CIS) with an Agilent Technologies gas chromatography system (GC), you had to use two methods and two sequences when analysing a set of samples. Users asked: Is there an easier way?

The software experts from GERSTEL came up with a great solution. “When you open ChemStation, you now find GERSTEL in the menu bar”, says Dr. Stefan Bobinger, chemist and software developer at GERSTEL. The menu item opens the GERSTEL MAster Software, which has recently been incorporated into the GC-ChemStation. In other words: „People no longer have to switch from one program to another to carry out their analyses“, says Dr. Bobinger. „The GERSTEL modules and GC can now be programmed using a single software package."

A mouse click selects the desired dialogue box to enter method parameters for all GERSTEL modules as well as choosing sample injection techniques such as TDS, SPME, headspace and liquid injection. The method parameters are stored together with the parameters for the GC-ChemStation. An extended sequence table allows choice of tray and injector.

„At last, things that belong together are together”, says Dr. Stefan Bobinger. He predicts: „In the near future, a similar software package will be available for MS-ChemStation users.“

GERSTEL ODP

with new speech recognition software

GERSTEL Olfactory Recorder Software

Classification of characterised aroma data in an „aromagram“ that are represented as different peak heights in the aromagram. The aromagram is then stored with data from any other detectors connected in parallel with the ODP 2. Pressing a key also activates the voice recording function and the aroma description spoken during that time is also stored along with the aromagram.

Once the olfactory analysis is completed, the spoken commentary can be reviewed, and corrected if necessary. A complete report can be generated that contains aroma detection times, descriptions and GC run information.

Italy: distributor with a new name

The Italian GERSTEL distributor has changed its name as part of a process of extensive internal corporate restructuring: Abreg s.r.l. has become A.I. Tech s.r.l. The company continues to be run by Roberto Gaita.
The GERSTEL Twister

**Stir Bar Sorptive Extraction (SBSE)** is a sample preparation technique developed at the Research Institute for Chromatography (RIC) in Belgium and is sold commercially as the GERSTEL Twister. The technique is comparable to Solid Phase Micro Extraction (SPME). The crucial difference between SPME and SBSE is that analyte extraction is accomplished using a much thicker phase (0.5 to 1-mm vs. 100-µm). For the Twister, this phase consists of pure polydimethylsiloxane (PDMS). The phase ratio—the ratio of the aqueous phase to the PDMS phase volume—is much lower for SBSE, and the recovery rate is thus higher. Extremely low detection limits can be achieved when compounds sorbed onto the Twister are transferred to the gas chromatograph by thermal desorption.

For the first time, we briefly describe how SBSE can be combined with liquid chromatography (HPLC). Analytes are extracted from the Twister using a small volume of acetonitrile (ACN) or an acetonitrile-water mixture. Aliquots of the resulting solution are then transferred manually to the HPLC system and analysed.

For the second time, we report on lecture tours in Japan and Korea. „Always 180 to 250 seminar attendees—informative discussions contracts—within a few days. The journey to Asia was a success.“ The plan of Andreas Hoffmann, Applications specialist at GERSTEL, and Prof. Dr. Pat Sandra from the Research Institute for Chromatography (RIC) Belgium, was to give talks in Japan and Korea with the aim to inform users about GERSTEL’s expanding product portfolio and recent scientific developments. Emphasis was placed on work performed at the RIC and at GERSTEL’s main laboratories in Germany using the GERSTEL Twister (SBSE). Eberhard G. Gerstel and Ralf Bremer, both Managing Directors, used the journey to visit key customers in Japan. „Our first impression was confirmed“, says Eberhard G. Gerstel. „GERSTEL is in greater demand than ever."

Four years ago, the company intensified its activities in Asia, especially in Japan. „The recession was at its worst then, and the economic situation has not improved much“, says the managing director and co-owner. „However, we have been able to provide analytical solutions that are in great demand. The name GERSTEL is becoming a key for users to solve their most difficult analytical problems."

GERSTEL has received excellent support from its Japanese business partner, Yokogawa Analytical Systems Inc. and its local representative, Dr. Manfred Schwarzer. „In summary, our trip achieved successes comparable to our recent trade shows“, says Eberhard G. Gerstel.

**Semi-automated determination of PAHs**

The GERSTEL Twister for sample preparation in HPLC

It is now possible to automate the SBSE desorption step and to transfer the liquid extract by means of a GERSTEL Multi Purpose Sampler MPS 3 to an HPLC system using a procedure developed at the UFZ Leipzig-Halle and marketed by GERSTEL. Called Twister Back Extraction, it requires an MPS 3 equipped with a temperature programmable agitator and special software.

There is only one manual step. The Twister must be removed by hand from the sample vial and transferred to a 250-µL glass insert located in a 2-mL sample vial. The MPS 3 adds the acetonitrile-water mixture, and transports the vial to the agitator. After it is agitated at a pre-set time and temperature, the vial is then removed and an aliquot of the solvent is injected into the HPLC system.

Combination of SBSE with solvent Back Extraction followed by LC fluorescence detection allows sensitive and reproducible determination of PAHs, pesticides, herbicides and phenols as well as many other non-volatile and thermally labile compounds in aqueous matrices. The Twister Back Extraction technique greatly reduces the manual labour involved when performing extractions. The procedure is also robust, easy to implement, and allows high sample throughput by extraction of many samples in parallel.

**RIC official distributor for Belgium**

The Research Institute for Chromatography (RIC) has been the official new GERSTEL distributor in Belgium since September 2002. The company has commissioned its previous representative, Analytical Application Britle B.V., to concentrate its operations on the Netherlands and England in particular.

**Further information**

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**GERSTEL on lecture tour in Japan and Korea**

> »In greater demand than ever.«

From food and beverages to environmental water and effluent analysis, and in numerous analytical laboratories, the GERSTEL Twister is increasingly used for extraction for volatile and semi-volatile analytes from aqueous matrices. With good reason:

When compared to SPME fibres, the Twister provides a much larger capacity. In addition, the PDMS functions as an immobilised liquid phase, in which the sample is concentrated by sorption not by adsorption. The combination of high capacity and sorptive extraction minimises or even eliminates competitive and displacement effects caused by highly concentrated matrix components.

Experiments were performed to confirm this:

The limits of sorption capacity of the Twister were determined gravimetrically by extracting hexadecane from aqueous isopropyl alcohol solutions. Under normal conditions, the PDMS phase of the Twister can absorb milligram amounts of hexadecane. From a practical point of view, the highest analyte concentration that gives a linear calibration curve, is the working range of the stirring bar.

For evaluation of the competitive and drag effects, model components, such as pesticides and methylesters, were extracted from water with the Twister and with SPME (also using a PDMS phase) in the presence of up to 5 ppm limonene.

Results: The PDMS phase of the Twister showed up to 25-fold higher capacity compared with the SPME phase.

Stir Bar Sorptive Extraction – Capacity Comparison
Aroma analysis of the finest

ChemSensor in research and routine

People follow their noses, and not only physically. Of all the senses, the sense of smell is the subtlest and controls us like no other. Bad smells startle us, and make us recoil. By contrast, we are drawn to pleasant smells and they can control our desires. For good reasons, aroma manufacturers devote themselves to keeping their formulations secret and try to find out others’ recipes through chemical analysis.

The GERSTEL Headspace ChemSensor is a special version of the GERSTEL ChemSensor that has been used successfully for classification of various fruit aromas. These aromas present a challenge for classification because they contain large amounts of propionaldehyde and ethanol that can interfere with the analysis. The Headspace ChemSensor consists of a headspace sampler directly coupled to a quadrupole mass spectrometer. The advantage of this configuration is that the analysis time is only three to four minutes per sample. Using multivariate data analysis, the data are classified by Pirouette pattern recognition software from Infometrix. Integration of the Headspace ChemSensor into routine analysis allows qualitative (classification) and quantitative (regression) analysis of various aromas.

For qualitative analysis, a multivariate analysis method, the algorithm of Soft Independent Modeling of Class Analogy (SIMCA) is used. SIMCA projection of the composite mass spectrum of an aroma sample can be represented as a point in a 3-dimensional space. The data (points) of similar aromas cluster together in the diagram; aromas with different volatile compositions are distributed over the entire diagram.

Quantitative determination is carried out using Partial Least Squares Regression (PLS). In predictive mode, the algorithm compares the mass spectrum fingerprint of unknown and known aroma samples. The ChemSensor was able to recognize differences in composition using the mass spectra fingerprints of aromas with true/false and yes/no classifications.

Conclusion: the results of aroma studies using the Headspace ChemSensor from GERSTEL can be used as objective guidelines in food processing, for quality control of starting materials as well as intermediate and finished products.

Efficient determination of the spoiling of food

Spoiled food contains substances that can be used as indicators of the degree of contamination, such as dimethyl sulphide in poultry and eggs, diacetyl in orange juice, or trimethylamine in fish and milk. Since the spectrum of volatile components alters with the degree of spoilage, it can be followed by determination of the amounts of these indicators. The GERSTEL ChemSensor has been shown to be the rapid and reliable method of choice for this type of analysis.

Many statistical methods can be used to develop a model for detection of indicators of spoilage. Explorative analysis methods, such as Principle Component Analysis (PCA) or Hierarchical Cluster Analysis (HCA) indicate the suitability of data for the classification modes. Soft Independent Modeling of Class Analogy (SIMCA) and the procedure known as K Nearest Neighbours (KNN) were used to develop two classification models. Regression models were found using partial least squares regression (PLS).

Results: Both SIMCA and KNN allowed rapid and secure identification of the foods noted above with and without spoilage indicators. The concentration of spoilage indicators was determined using PLS models to be in the lower and middle ppm ranges. The ChemSensor allows rapid and reliable determination of spoilage indicators and thus signs about the degree of spoilage.

Conclusion: use of the Headspace ChemSensor for classification because they contain large amounts of propionaldehyde and ethanol that can interfere with the analysis.

Classification of coffee varieties with the ChemSensor

Consistent quality is a basic requirement for long-term client relationships – in the case of luxury foods, aroma can be a significant part of the product’s appeal, and this is particularly true for coffee. The distinctive aroma of various varieties of coffee and mixtures must be maintained. How can we classify coffee varieties rapidly and reliably in order to be able to produce a variety of products with consistent quality and aroma?

To answer this, simultaneous, semi-quantitative steam-distillation extraction gas chromatography with mass-selective detection (SDE-GC-MS), a technique commonly used in the coffee industry, was compared with the results obtained using the GERSTEL Headspace ChemSensor System. The latter is an electronic nose, using quadrupole mass spectrometry and Headspace sampling.

Using SDE-GC-MS, taste analysis was carried out with freshly roasted and ground green coffee beans, using Arabic and Robusta varieties. Principle Component Analysis (PCA) showed a clear difference between the two varieties. Furthermore, the Arabica variety gave a cluster corresponding to its sensory descriptors—confirming the good correspondence between sensory and chemical analysis data.

Intermediate results: while classical SDE-GC-MS permitted good classification, it was very time consuming (total analysis time per coffee sample: 6 h of which 4 h for SDE).

Measurement using the Headspace ChemSensor System, in which the results were analysed using special pattern recognition software showed the coffee varieties successfully classified, but in a much shorter time.

Conclusion: use of the Headspace ChemSensor Systems from GERSTEL is an effective alternative to classical SDE-GC-MS in classification of coffee varieties.

**ChemSensor confirms the authenticity of whiskey**

Headspace technique and GERSTEL Twister combined

Sometimes food QC departments have real trouble confirming the authenticity of a product. For example, alcoholic beverages such as bourbon can be adulterated by addition of caramel colouring and water or by adding a lower quality whiskey. With a little skill you can create what the inexperienced consumer will perceive as drinkable bourbon. Experts can tell the difference in taste. However, a taste test is not on the same level as a statement such as, “the probability limits are …”. Authentic or fake? A new procedure sheds light.

Several bourbons were analysed with GERSTEL Headspace ChemSensor with mass-selective detection. Sampling was carried out using the headspace injection technique. For validation of the results and classification of which individual components are relevant, the samples were also analysed using the GERSTEL Twister (Stir Bar Sorptive Extraction) technique.

Results: with the aid of multivariate analysis techniques such as Soft Independent Modeling of Class Analogy (SIMCA) and Principle Component Regression (PCR), the blended bourbons were successfully identified. Blending with cheap bourbons or other adulterants adds traces of new components and allows the term “bourbon” to be classified as a blend and not authentic; classification models for both sample preparation techniques confirmed the results. In particular, SBSE allowed identification of components that were not found using the headspace sampling technique (HS). Identification of blended bourbons by a combination of HS and SBSE can be seen as confirmation of the versatility and applicability of the GERSTEL ChemSensor for rapid, precise and accurate differentiation of samples with similar chemical compositions.

It’s quicker ...

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Conclusion: use of the Headspace ChemSensor Systems from GERSTEL is an effective alternative to classical SDE-GC-MS in classification of coffee varieties.
Dr. Bobinger, can you tell us how the idea of two MPS one on top of the other, came about? As with many of products and product enhancements, GERSTEL was asked by a customer to help them with their special sample preparation needs. Our solution of using two MPS 2 samplers and customised software, the GERSTEL PrepStation, fulfilled this need. We see an enormous need for more sophisticated sample preparation packages that the PrepStation will be able to address.

What is the advantage of two Multi Purpose Samplers placed one on the other? The functionality of one sampler is very limited with sample preparation is still the most time consuming and critical part to providing high quality qualitative or quantitative sample analysis. This is not going to change. However, time and expense can be reduced, and manual steps can be automated. GERSTEL is in a great position to provide new levels of sample preparation with the MPS PrepStation. Why configure an instrument with more than one sampler? GERSTEL Solutions worldwide in conversation with chemist and co-developer Dr. Stefan Bobinger.

The lab, endless work. Here we are in 2002 - and users still have to cope with the fact: sample preparation is still the most time consuming and critical part to providing high quality qualitative or quantitative sample analysis. This is not going to change. However, time and expense can be reduced, and manual steps can be automated. GERSTEL is in a great position to provide new levels of sample preparation with the MPS PrepStation. Why configure an instrument with more than one sampler? GERSTEL Solutions worldwide in conversation with chemist and co-developer Dr. Stefan Bobinger.

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