

**GERSTEL**

solutions  
worldwide

ISSN 1619-0076

News from GERSTEL GmbH & Co. KG · Aktienstraße 232 – 234 · D-45473 Mülheim an der Ruhr · Germany · Phone +49 (0) 208 - 765 03-0 · Fax +49 (0) 208 - 765 0333

**GERSTEL in Show Year 2002**

# More time for important things



**GERSTEL Network**

Our distributors in the  
Netherlands and Italy



**Analysis**

Trace analysis of taints  
in foods and beverages



**Formaldehyde Analyzer**

Determination in materials  
parallel to GC



**Ralf Bremer**

Technical director  
of GERSTEL  
GmbH & Co.KG

# GERSTEL solutions: More time for the essentials ...

GERSTEL's analytical solutions give you the power to solve the most challenging problems while allowing you to easily adapt to future needs. GERSTEL's approach is to listen carefully to our customers and to provide them with superior solutions. This customer-oriented systems design philosophy means that the GERSTEL solution is comprehensive, encompassing engineering, applications development, and full instrument support. Our modular systems approach allows you to expand your capabilities as your needs evolve, thus assuring your investment for the future.

We invite you to visit with us in the GERSTEL exhibits at PittCon 2002 in New Orleans and at Analytica 2002 in Munich. We have some important and exciting new analytical solutions to share with you, including:

- Our new ChemSensor product line combines technologies from three world leaders: Agilent Technologies quadrupole mass spectrometry, Infometrix multivariate chemometrics, and GERSTEL sample conditioning and automation. The new ChemSensor offers important advantages over conventional electronic nose products.

- New developments with our TDS thermal desorption systems, MPS multi-purpose samplers, and Twister Stir Bar Sorptive Extraction systems that provide even better performance, greater versatility, and productivity-enhancing automation for a wide range of applications.

- Further optimization and enhanced performance of our CIS Cooled Inlet System, which has already proven itself more than a thousand times over!

We think that you will find a visit to the GERSTEL booth to be well worthwhile. The GERSTEL team looks forward to meeting with you.

Yours truly,

*Ralf Bremer*

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worldwide business

Smoke Analyzer

**Strong partner with synergy potential**

# Agilent Technologies and GERSTEL

**Agilent Technologies**  
Innovating the HP WayPremier Solution Partner  
Gold Level

The decision of Agilent Technologies Inc. to transfer worldwide trading, support and further development of the ChemSensor 4440 to GERSTEL indicates a new closer relationship between the two companies. Both have recognised the enormous synergy potential for more than 15 years: That is, GERSTEL systems specifically designed for use with Agilent Technologies instruments will open new markets and offer complete »off the shelf« solutions to customers through out the world.

GERSTEL solutions include the Air Monitoring System (AMS), consisting of two 6890s with GERSTEL TDS G, Easy Cut and CTS 3 for online air monitoring of polar and non-polar components during a GC run.

Another is the smoke analyzer, specially developed for the study of cigarette smoke and realised using two coupled GC 6890s from Agilent Technologies with the GERSTEL CTS 1 and two mass-selective detectors.

The importance to Agilent Technologies of the partnership is shown by the title awarded to GERSTEL:

Premier Solution Partner – Gold Level.

Air Monitoring System  
AMS

## Infometrix Inc. and GERSTEL

Infometrix is one of the leading software developers for chemometry in the world. Since 1978, the company has been developing chemometric tools, which can be used alone or employed in numerous chemometric solutions. An Infometrix product based on Pirouette and developed exclusively for GERSTEL controls the ChemSensor 4440 and the ChemSensor System 4440 and validates the results.

Differentiating between different colas (regular or diet), determining the ratio of components in diesel fuel, or determining the origin of an olive oil are simple tasks for the ChemSensor 4440. This is all made possible by the wide variety of algorithms available in the software designed by Infometrix.

**GERSTEL  
ChemSensor  
System**

Infometrix software classifies a sample using different algorithms

## OI Corporation and GERSTEL

A promising link. This is the conclusion of the OI Corporation, manufacturer and retailer of numerous products for gas, ion, and gel permeation chromatography. With good reason: while OI is mainly concerned with the detection side of chromatography, GERSTEL concentrates on sample preparation. It seemed an obvious step to cooperate and to expand. Since the

end of last year, GERSTEL has been the exclusive sales and support provider for OI Corporation detectors and GC systems in the German speaking portion of the world.

Further  
informationGERSTEL: [www.gerstel.com](http://www.gerstel.com)Agilent Technologies: [www.agilent.com](http://www.agilent.com)OI Corporation: [www.oico.com](http://www.oico.com)Infometrix: [www.infometrix.com](http://www.infometrix.com)

**GERSTEL service and support network: Our Distributor in Benelux and UK**

# Analytical Applications Brielle B.V.

Since 1991, Analytical Applications has been involved in specialist application-support for analytical laboratories. We are a »Value Added Business Partner« of Agilent Technologies, GERSTEL and other vendors. In close cooperation with our contract partners we concentrate on the field of GC, HPLC, GC/MS and LC/MS applications.

The offices of Analytical Applications are located in Brielle, The Netherlands, and Farnborough, United Kingdom (U.K.). Our Dutch office has recently moved into a new building with brand new facilities including a separate seminar area equipped for classroom training, a spacious application lab, and storage space allowing instruments for rental and leasing programmes to be dispatched to the customer immediately from stock. The offices are thus perfectly designed to handle the major business activities of Analytical Applications: System Integration, Rentals & Leases and Support Services. The U.K. office has recently cooperated with the Food Research Institute in Leatherhead, and a report on this also appears in this issue.

Doing business with Analytical Applications means doing business with an enthusiastic experienced team, giving personal service and advice. Our Sales Departments, in both The Netherlands and the U.K., offer clients advice and integrated analytical solutions. The Sales Department is complemented by Support Services, looking after installations, maintenance and repairs and training. All telephone calls and orders are processed immediately by our administrative staff.



**Karel Lund**  
Director of Analytical  
Applications Brielle B.V.

## The staff

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Frank van Schooten  
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Fanina Zwart  
(Order Processing),  
Jeroen Weijts  
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## System Integration

Through close cooperation with Contract Partners such as GERSTEL, Analytical Applications offers the customer multi-vendor solutions and therefore complete system integration. For the customers this results in a so called One-Stop-Shop.

## Rentals & Leases

Renting & Leases GC, GC/MS, LC or LC/MS systems, including full service, can be the ideal solution in case of limited budget availability or emergencies. The equipment is immediately available from stock. After renting the equipment for 1 to 12 months, the system can be purchased or returned.

## Support Services

After thorough consultation about the application, systems are specifically tailored for and demonstrated to customers in the modern laboratory by Analytical Applications' own Applications Chemists. Installation, training and maintenance of the equipment is provided by the Support Engineers. In addition to technical consultancy, the Support Department also provides demonstration workshops and training in analytical instrumentation.

## Market Segments

The market segments Analytical Applications serves and will continue to serve from its new premises, are predominantly in the fragrances, food and pharmaceutical industries. In addition we are active in the areas of chemical, petrochemical, agricultural, environmental and pyrolysis applications.



## Let's twist again

# Trace analysis of taints in foods and beverages using Stir Bar Sorptive Extraction (SBSE)

## Authors

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## Introduction

Stir Bar Sorptive Extraction (SBSE) is a novel technique for sample extraction.<sup>1, 2</sup> Analyte extraction is based on a small glass stir bar (10 or 20 mm in length) coated with a 1 mm thick layer of polydimethylsiloxane (PDMS). The 10 mm SBSE has a PDMS volume of 24  $\mu\text{L}$ , which compares with an solid phase micro extraction (SPME) fibre, typically coated with less than 0.5  $\mu\text{L}$  of adsorbent. Within the glass bar is a metal strip to enable magnetic stirring. After sampling, the stir bar is removed, washed and placed in a thermal desorption unit. The analytes are thermally desorbed by heating and determined by GC-MS.

This work describes a comparative study on the analysis of contaminating compounds associated with taints in foods and beverages based on SBSE and SPME. The presence of contaminants resulting in organoleptic problems of off-odour and taint in food products can result in considerable economic loss to a manufacturer in terms of sales and product reputation.

The first study compares the analysis of a „cocktail mixture“ of 11 volatile compounds commonly associated with problems of taint in foods and beverages. The second involves the analysis for halophenols and haloanisoles in water and alcoholic beverages.

## Experimental

### Instrumentation

All analyses were performed on a GC (6890 Agilent Technologies) with mass selective detection (5973 Agilent Technologies). For SBSE analysis, the GC was equipped with a Thermal Desorption unit (TDS 2, GERSTEL), and a cooled injection system (CIS 4, GERSTEL). For SPME analysis, the PDMS (100 mm) fibre was desorbed directly in the CIS 4, configured for operation as a GC injector.

### Cocktail mixture

Standards were prepared by spiking 11 compounds into water. The water had been previously boiled and cooled to removing residual volatiles. Sampling was undertaken on 10 mL aliquots for 30 min at ambient temperature (20 °C). Desorption from SPME fibre and SBSE stir bars were undertaken at 200 °C. The GC-MS analysis was undertaken using a 30 m x 0.25 mm i.d.,

## GERSTEL- Twister

In combination with GERSTEL TDS for the determination of flavour and off-flavour compounds

0.25 mm film thickness HP5 column, with a temperature program of 50 °C (2 min) – 10 °C/min – 220 °C. The MS was set to scan mass range 40-300 m/z.

## Halophenols and haloanisoles

Samples of water, wine simulant (10 % ethanol) and white wine were spiked with the following: 2,4,6-trichloroanisole (2,4,6-TCA), 2,4,6-trichlorophenol (2,4,6-TCP), 2,4,6-tribromoanisole (2,4,6-TBA) and 2,4,6-tribromophenol (2,4,6-TBP), at levels corresponding to 0, 0.001, 0.01, 0.1 and 1 ppb ( $\mu\text{g}/\text{mL}$ ). Each sample was also spiked with 2,3,6-trichloroanisole (2,3,6-TCA) and 2,3,6-trichlorophenol (2,3,6-TCP) at 0.1 ppb ( $\mu\text{g}/\text{mL}$ ) as internal marker standards.

Sampling was undertaken on 10 mL aliquots for 30 min at ambient temperature (20 °C). Desorption from SPME fibre and SBSE stir bars was undertaken at 280 °C and 220 °C, respectively. The GC-MS analysis was undertaken using a 30 m x 0.25 mm i.d., 0.25 mm film thickness HP5 column, temperature programmed 120 °C (1 min) – 3 °C/min – 200 °C. The MS was set to monitor the following 8 mass ions (195, 210, 196, 198, 330, 332, 344 and 346 m/z) as a single group. The mass ion dwell time was 80 milliseconds.

## Results and Discussion

### Cocktail mixture

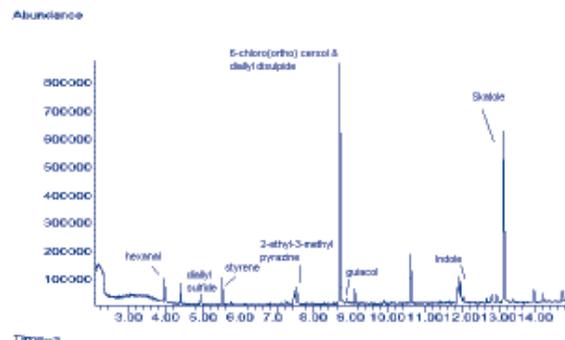
The responses of 11 components of „cocktail mixture“ analysed by SPME-GC-MS and SBSE-GC-MS were determined. Based on mass ion peak area measurements from RIC data, comparison of analyte level of responses by SPME headspace and direct immersion SBSE analyses (spiked at 10 ppb) can be made (Table 1).

The SBSE GC/MS (tic) chromatogram for taint cocktail mix (10 ppb spike) in water is shown in Figure 1.

**Table 1**  
Relative SBSE response compared with SPME for „taint cocktail mix“ compounds

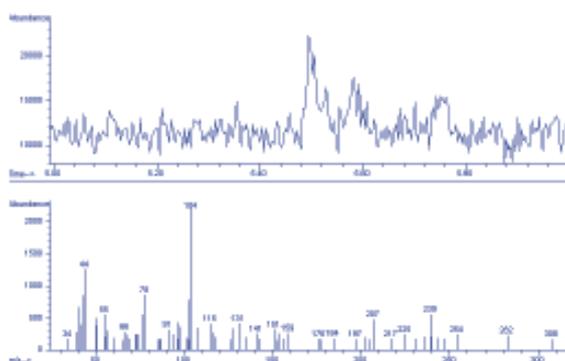
Compound	Retention time (min)	Molecular mass ion (m/z)	Ratio
Allyl methyl sulphide	2.8	88	*
Hexanal	4.0	82	6.4
Diallyl sulfide	4.9	114	0.7
Styrene	5.5	104	1.5
2-Ethyl-3-methyl pyrazine	7.4	122	24.6
m-Cresol	8.5	108	*
6-Chloro(ortho) cresol (6-COC)	8.6	142	8.0
Diallyl disulfide	8.6	146	4.9
Guaiacol	8.8	124	18.1
Indole	11.9	117	103.6
Skatole	13.2	131	202.2

\* not detected.



**Figure 1**

SBSE GC/MS (tic) of taint cocktail mix (10 ppb) spiked in water



**Figure 2**

SBSE GC/MS analysis of styrene (10 ppb) spiked in milk

Overall, the data show that, for the majority of compounds, a higher response value was obtained with SBSE than with SPME. Higher levels of extraction can be seen for less volatile components such as indole and skatole, which gave at least a 100-fold improvement in the level of response.

Investigation of the detection of the „taint cocktail mix“ spiked in milk was also undertaken. Based on definitive mass spectra data, the following compounds were identified at a 10 ppb (10  $\mu\text{g}/\text{mL}$ ) spiking level: hexanal, styrene, 2-ethyl-3-methylpyrazine, 6-chloro (ortho) cresol (6-COC), diallyl disulfide, indole and skatole. The mass spectra of styrene and 6-COC are shown, respectively, in Figure 2 and 3. Figure 3 also shows the RIC for the molecular ions of 6-COC (142 m/z) and the coeluting diallyl disulfide (146 m/z).

## Halophenols and haloanisoles

Water, wine simulant (10 % ethanol) and white wine samples were spiked with 2,4,6-TCA and 2,4,6-TCP at levels of: 0, 0.001, 0.01, 0.1 and 1 ppb ( $\mu\text{g}/\text{mL}$ ). 2,3,6-TCP and 2,3,6-TCA were added as an internal marker standard (0.1 ppb).

**Table 2**

Correlation coefficient ( $r^2$ ) values for halophenols and haloanisoles spiked in different matrices

Matrix	2,4,6-TCP	2,4,6-TBP	2,4,6-TCA	2,4,6-TBA
Water	0.9944	0.9995	0.9996	0.9985
Wine simulant	0.9994	0.9933	0.9971	0.9972
Wine	0.9976	0.9961	0.9995	0.9917

Under the analytical conditions used, 2,4,6-TCA and 2,4,6-TBA were detectable in water, wine simulant and white wine at 10 ppt spiking level by SBME GC/MS (Fig. 4). 2,4,6-TCP and TBP were also detectable at this spiking level in water and wine simulant. However, although 2,4,6-TBP was detectable at 10 ppt spiking level, owing to co-eluting interferences 2,4,6-TCP was not detectable in white wine at this spiking level.

Figure 5 shows the corresponding GC/MS SIM mass ion chromatograms for 2,4,6-trichloroanisoles/phenols, spiking at a 10 ppt level sampling by direct immersion SPME. The 2,3,6-TCA internal marker standard (0.1 ppb) is the only component detected. 2,4,6-TCP and 2,4,6-TBP were detectable by SPME (direct immersion) in samples spiked at 1 ppb (Fig. 6).

The studies show that detection of haloanisoles (i.e. 2,4,6-TCA and 2,4,6-TBA) in the above matrices is improved ten-fold when sampling by SBSE compared with SPME, where the fibre is directly immersed in the aqueous matrices. In the case of halophenols (i.e. 2,4,6-TCP and 2,4,6-TBP), the level of detection by SBSE was of the order of 10 ppt. This was 100 times better compared with direct immersion SPME (i.e. 1 ppb).

Regression data show that the calibration curve for halophenols and anisoles at the sub parts per billion level (0-1000 ppt) is linear. The correlation coefficient values ( $r^2$ ) for halophenols and anisoles are given below (Table 2).

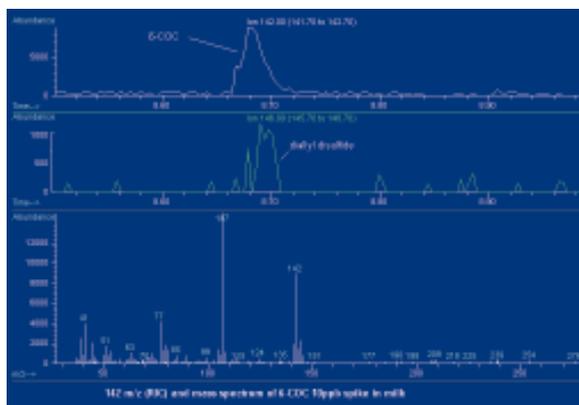
## Conclusions

SBSE is a rapid and easy method for determining tainting compounds in aqueous foods and beverages. This study has demonstrated the applicability of sampling at the low and sub part per billion levels for tainting contaminants. The results show that, for certain contaminants, the level of detection can be improved by a factor of at least 100 compared with sample extraction by direct immersion solid phase micro extraction (SPME).

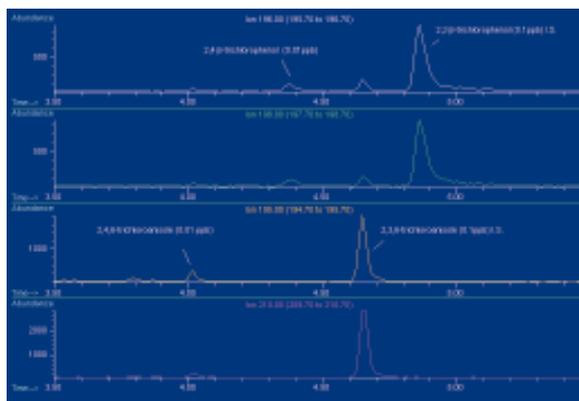
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[1] Baltussen E, Sandra P, David F and Crammers C, „Stir Bar Sorptive Extraction (SBSE), a novel extraction technique for aqueous samples theory and principles“, *Journal of Microcolumn Separations*, September, 1999, 11, 737-747.

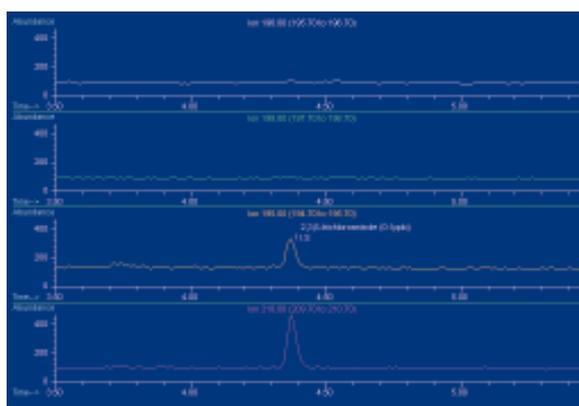
[2] Hoffmann A and Heiden A, „Determination of flavour and off-flavour compounds in dairy products using Stir Bar Sorptive Extraction (SBSE) and thermal desorption GC/MSD/PFPD“, *App Note 5/2000, Gerstel, 2000.*



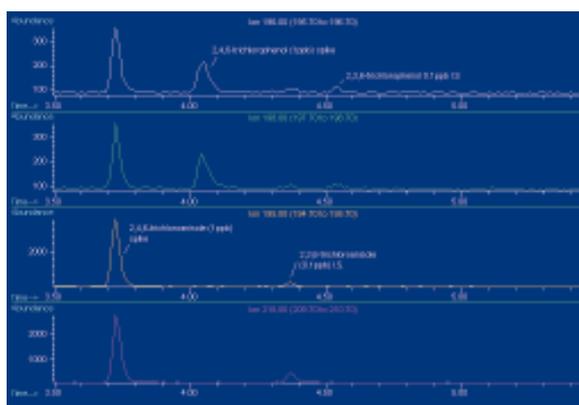
**Figure 3**  
SBSE GC/MS analysis of 6-COC (10 ppb) spiked in milk



**Figure 4**  
SBSE GC/MS analysis of 2,4,6-trichlorophenols/anisoles (0.01 ppb) spiked in water



**Figure 5**  
SPME (direct immersion) GC/MS analysis of 2,4,6-trichlorophenols/anisoles (0.01) ppb spiked in water



**Figure 6**  
SPME (direct immersion) GC/MS analysis of 2,4,6-TCA/TCP spiked at 1 ppb level

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## ChemSensor System

## Electronic nose based on MS

Numerous business areas are increasingly using electronic noses for quality assurance, and in monitoring products and processes. From the small group of market-ready systems, one stands out: the GERSTEL-ChemSensor 4440. The instrument has been used successfully for more than three years, mainly in monitoring production lines for sensory determination of volatile headspace components. A crucial difference determines

success: in contrast to conventional electronic noses, the ChemSensor 4440 does not work with relatively solid state sensors, but is based on quadrupole mass spectrometry technology. The headspace volatiles are transferred directly to the mass selective detector (MSD) with elective scan mass ranges resulting in fast analysis time. The resulting mass spectrum is used as a fingerprint to train the ChemSensor with acceptable samples.

Products that do match this fingerprint are easily recognized. For example, for qualitative analysis a simple good/bad output could be used. For quantitative analysis measurement of component content could be made using percentage terms. Differences between samples are also found using the GC/MS configuration, which is ideal for R&D applications. Discriminating ions previously determined with the 4440 can be searched in the GC/MS and the differentiating compounds could easily be found.

ChemSensor software developed exclusively for the GERSTEL ChemSensor 4440 by Infometrix Inc. allows the visualization of these mass spectra with pattern recognition techniques. The software is capable of controlling the hardware as well as creating chemometric models in an integrated package.



### **GERSTEL ChemSensor 4440**

Based on well-known mass spectrometry quadrupole technology.

**Now also for passive sampling tubes**

## Thermo Desorption System TDS 2-7

The Thermo Desorption System TDS 2 product family from GERSTEL has grown: thanks to a change in the internal dimensions of the heating chamber, the new TDS 2-7, besides using the standard TDS tubes from GERSTEL, allows use of thermal desorption based passive sampling tubes in sizes 1/4" x 3.5" from other manufacturers for the first time. Automation was accomplished by modifying the proven TDS A with a new microprocessor controlled tube lift mechanism designed to easily handle the different tube sizes. The mechanical lift was replaced by a microprocessor controlled lift arm.



### **GERSTEL TDS 2-7**

First time for thermal desorption based passive sampling tubes in sizes 1/4" x 3.5" from other manufacturers

### **Standard Gas Preparation System SPS**

## Individual calibration gases

The patented dynamic Standard Gas Preparation System SPS from GERSTEL allows rapid and cost-effective production of any desired gaseous calibration mixture for thermal desorption. The system (currently

undergoing final testing) is an alternative to calibration gas mixes stored in gas cylinders. Until now, these have been the best, but most expensive sources for calibration gas mixtures. Because of production-related long supply times for individual gases, many users have stopped using these sources. Besides this, some mixtures are not commercially available because they are not stable in pressurised gas

containers. The precision and accuracy of the SPS is possible thanks to a piezocrystal controlled microdrop system – also used in colour inkjet printers – the individual drops of the calibration solution are sprayed at a precisely defined rate into a highly purified gas stream (N<sub>2</sub> or air); the process is carried out under normal pressure. Because of the small drop diameter of 30 to 60 µm, the components vaporise completely. By controlling the frequency, the piezocrystal allows injection of 1 to 2000 drops per second with a volume of approximately 15 picolitres (10<sup>-12</sup> L) into the gas stream: the digitally determined drop frequency allows calibration over three orders of magnitude – with no mechanical changes to the system or changes in the gas flow.



### **Cooled Injection System CIS 6**

## Heating to 600 °C for the first time

The product range of the most frequently used universal injectors for all tasks in gas chromatography has been extended. In addition to the current GERSTEL Cooled Injection Systems (the CIS 3 and CIS 4), two new versions will be available soon. The CIS 6 is the new universal injector designed specifically for Agilent Technologies' 6850 and 6890 gas chromatographs, and the CIS 5 is for use in other manufactures' gas chromatographs. The new CIS inlets have been improved through the optimization of construction and improved heating technology. For the first time they offer programmable heating to 600 °C. The new inlets will come with a choice of LN<sub>2</sub>, LCO<sub>2</sub>, Peltier or cryostatic cooling.



### **GERSTEL CIS 6**

Designed for the Agilent Technologies 6850 and 6890 gas chromatographs

**GERSTEL is  
there for you.**

### March

#### LifeCom 2002

Heinrich Heine Universität  
Düsseldorf, Germany,  
from 12. to 14.03.2002

#### Pittcon 2002

New Orleans, USA,  
from 17 to 21.03.2002

#### ForumLabo 2002

Paris, France,  
from 26. to 29.03.2002

### April

#### PALAB

Fa. Novartis,  
Basel, Switzerland,  
from 08. to 09.04.2002

#### ANALYTICA 2002

Neue Messe München,  
Germany,  
from 23. to 26.04.2002

### May

#### 25<sup>th</sup> International

Symposium on  
Capillary Chromatography  
Riva, Italy,  
from 13. to 17.05.2002

### June

#### Institute of

Food Technologists (IFT)  
Anaheim, USA,  
from 15. to 19. 06.2002

### August

#### American Chemical Society (ACS)

Boston, USA,  
from 18. to 22. 08.2002

### September

#### Analytica China 2002

Shanghai, China,  
from 03. to 06.09.2002

#### Japan Analytical Instruments Manufacturers Association (JAIMA)

Japan,  
from 05. to 07.09.2002

### November

#### Het Instrument

Utrecht, The Netherlands,  
from 04. to 08.11.2002

## MultiPurposeSampler MPS 2 and 3: New features for the MPS family

# Twister option for MPS 2

Save time and money when using gas chromatography. With this in mind, GERSTEL concentrated on developing a simple desorption unit for the Twister, a patented stir bar with a PDMS coating. With the Twister, organic components can be extracted from any aqueous matrices rapidly with up to 1000 times lower detection limits than SPME.

As a result of its efforts, GERSTEL is now in the final stages of testing the Twister



## Twister Desorption Unit TDU

The combination with MPS 2 for desorption of the Twister is an alternative to the TDS 2 plus TDS A

Desorption Unit (TDU). The TDU is based on the same principle as the very successful TDS 2, but is significantly smaller with a thermal desorption oven designed specifically for the Twister. Automation of up to 200 Twister analyses is made possible by simply using an adaptation kit for the GERSTEL MPS 2.

# Twister Back Extraction for the MPS 3

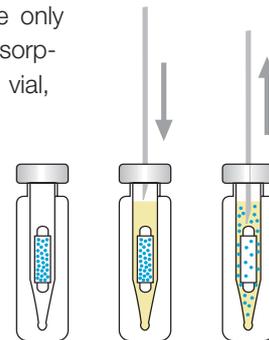
Back extraction using Twister is the first method to automate the SBSE liquid desorption step of the Twister, and to inject the liquid extract with the aid of the Multi Purpose Sampler MPS 3 directly into a HPLC system. This requires using 250 µL vials and the sample preparation option of the GERSTEL MASTER software. This allows complete flexibility of MPS 3 control for method development.

A case study: for enrichment of PAHs, 10 mL of the water sample to be investigated are placed in a 10 mL glass vial, containing the Twister. It is extracted for about 60 minutes at 100 rpm at room temperature. The Twister is then removed from the vial using clean forceps, dried with a lint-free wipe, and transferred in a conical glass insert to a 2 mL sample vial, which is closed with a magnetic cap or a plastic screw cap with an applied

metal ring. Usually, this is the only manual step; addition of the desorption solution, shaking of the vial, removal and injection of the extract occur automatically.

The combination of the Stir Bar Sorptive Extraction (SBSE) with solvent desorption followed by LC fluorescence detection allows sensitive and reproducible

determination of PAHs in aqueous samples. Thanks to the MPS 3, manual steps are greatly reduced. The procedure is robust and easy to carry out. Samples can be extracted in parallel, automatically processed and analysed, giving higher sample throughput. The Back extraction with Twister can be used for other organic compounds, such as the determination of pesticides, herbicides and phenols.

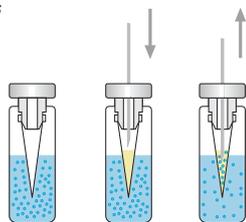


# Membrane Extraction for the MPS

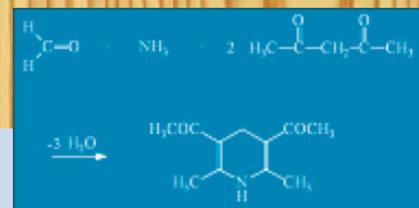
Thanks to the new membrane extraction, even dirty aqueous matrices can be studied chromatographically without numerous sample preparation steps. The functional principle of membrane extraction is based on a physical mechanism: the distribution between two phases corresponds to the distribution

coefficients combined with the exchange between the two phases through a permeable membrane.

In detail: the sample is transferred to a 20 mL headspace vial and sealed. The vial cap contains a membrane which will be filled automatically by the MPS with an extraction solution. After a suitable exchange time with support by heating and shaking the vial in the agitator, the organic components are enriched in the solvent phase depending upon their distribution coefficients; the MPS takes an aliquot and injects it into the GC or HPLC – automatically.



You can find further information on times, services and products on our internet home page at [www.gerstel.com](http://www.gerstel.com)



## Formaldehyde Analyzer

# Determination in materials parallel to GC

Determination of the formaldehyde concentration in materials has until now been carried out photometrically after extraction and derivatisation with acetylacetone in aqueous solution. Liquid gas chromatography determination of formaldehyde could only be performed after extraction and derivatisation, and so liquid chromatography using UV/VIS or fluorescence detection has been preferred; the derivatisation is carried out according to DIN 53315 at acidic pH with 2,4-dinitrophenylhydrazine in acetonitrile.

The automobile, furniture, packaging and food industries predominantly use the so-called flask method (VDA recommendation 275 / DIN EN 717-3): in a chamber atmosphere, released formaldehyde enriches an aqueous solution until equilibrium is achieved, and the formaldehyde is determined after derivatisation with acetylacetone.

Besides formaldehyde, the whole spectrum of volatile organic compounds in a material, or its emission spectrum, is usually also of interest. Thanks to the combi-

The working range so far established statistically for determination of formaldehyde with the formaldehyde analyzer is a total of 10 ng to 100 ng. However, the linear range extends to more than 1000 ng (1 µg). With material contents according to VDA 278 the following working ranges, related to the material, can be used analytically:

Another advantage of the formaldehyde analyzer is the low cross-reaction, such as to phenol, as observed with the flask method (see Table 2). In order to discover the extent to which formaldehyde measurement with the formaldehyde analyzer is affected by cross-reaction with phenol, aqueous standard solutions containing increasing concentrations of phenol were prepared and measured. The same solutions were determined photometrically with the acetylacetone procedure according to VDA 275. The results of the measurements with both methods are compared in the Table 2.

## Appendix

AERO-Laser and GERSTEL started cooperating this year to study formaldehyde emissions from materials directly using thermal extraction in addition to other liquid organic compounds. The result of this cooperation is a special adaptation of the AERO-Laser AL 4021 Formaldehyde analyzer to GERSTEL Thermo Desorption Systems, which is marketed by GERSTEL. By adaptation of the formaldehyde analyzer to the GERSTEL Thermo Extractor, the pure formaldehyde emission of a material can be measured simply without sample preparation. This work was carried out by Dr. Hans-Peter Schlegelmilch at imat-uve in Neuss, who largely managed this project.

**Figure 1**

Reaction of formaldehyde with acetylacetone and  $\text{NH}_3$  in an aqueous phase forming a-a'-dimethyl-b-b'-diacetylpyridine.

**Table 1** Working ranges

Material	Recommended contents according to VDA 278	Working range µg / g
Foam / leather / varnish	15 mg	0.67 – 66.7
Compound materials / foil-like materials	30 mg	0.33 – 33.3
Fibre compound materials	60 mg	0.17 – 16.7

nation of a GERSTEL Thermo Desorption System TDS 2 with GC-MSD and the parallel use of the Formaldehyde Analyzer from AERO-Laser, Garmisch-Partenkirchen, Germany, the emission potential according to VDA 278 from the material being studied can now for the first time be measured directly using thermal extraction.

In detail: the selective detection of formaldehyde is based on the reaction of formaldehyde with acetylacetone and  $\text{NH}_3$  in aqueous phase. This leads to formation of a-a'-dimethyl-b-b'-diacetylpyridine, which is excited at 400 nm (Hg lamp) and detected at 510 nm in the fluorescence cell (Figure 1).

The gaseous formaldehyde from the CIS split exit is mixed in a strip cell with the reaction solution with defined flow rates and contact times. Gas and reaction solution are separated at the exit from the cell, and the solution is led to the fluorescence measurement cell.



## The Author



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**Table 2**

Cross-reaction with phenol after normalisation of measurement without interference (without phenol addition) to 500 µg/L.

HCHO concentration [µg/L]	Phenol addition [µg/L]	Combination: TDS 2 / GC-MSD / Formaldehyde Analyzer [µg/L]	UV-VIS VDA 275 [µg/L]
500	0	500	500
500	10	499	514
500	50	498	508
500	500	493	522
500	5000	490	523
500	50000	493	525
500	500000	494	540
500	1000000	495	557

# User's Guide for CIS and TDS



The GERSTEL Thermo Desorption System TDS 2 (in all its available forms) is an extremely sensitive thermal desorption system. It can be used for classical thermal desorption or for direct thermal extraction without sample preparation. The GERSTEL Cooled Injection System CIS is the most frequently used septum-less sampling head in the world for all injection techniques in gas chromatography: split, splitless, on-column, large volume up to 1000 µL.

For both systems, the first edition of a compact user's guide is available in booklet form, describing the procedures and possible uses. The texts are short and concise; numerous tables and figures enable rapid understanding and thus make it easy to convert basic theory into practice.

## GERSTEL service and support network

# Our Distributor in Italy: ABreg S.r.l.

During the last quarter of 1999 we started to work on the idea of pooling our professional experience in a common plan, which has found its own shape and motivation in ABreg. Each of the founders has had a long career in sales and assistance in the field of analytical devices distributed by HP then Agilent Chemical Analysis Group.

The aim that sustained our project was to fulfil the ever-increasing number of requests and requirements

## Further information

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of customers for instruments able to provide global solutions. For this reason we searched for a company that could offer its own instruments with Agilent high compatibility.

GERSTEL was a natural choice because of the strong long-term partnership. In Twister we saw great potential for success, and for the last year

we have progressively been introducing GERSTEL to the Italian market. The promotional initiative for GERSTEL products has resulted in ABreg giving a number of demonstrations where real samples of different types supplied by customers have been examined.

We have had a high success rate with the »demos« and many potential customers who visited us

with their samples have now adopted GERSTEL solutions. In certain specific cases we promoted Agilent to increase sales of their products further.

Our experience has increased rapidly, and our sales staff has details of more than 80 analyses performed on different kind of samples.

Analyses of pesticides contained in food products performed using Twister were found to be highly sensitive and reproducible, as well as easy to use. As we approach the end of our first year as a GERSTEL distributor, we are looking forward to new challenges in the future, after the great successes of the past year.



### ABreg represents GERSTEL

At the most important analytical exhibition in Italy (Milan) in October 2001



# Determination of Herbicides in Vegetables

## Author

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## Introduction

A carrot obtained from a supermarket chain was analysed in order to detect herbicides by means of a classic method of solvent extraction, purification on a silica gel column, concentration under vacuum and analysis by GC-MS.

The sample turned out to contain 52 ppb of Trifluralin (alpha, alpha, alpha-trifluoro-2,6-di-nitro-N,N-dipropyl-p-toluidine, CAS number 001582-09-8), a well known herbicide, which may be absorbed by carrots if used incorrectly, excessively or if the latency time is not observed.

The same sample was used to evaluate the SBSE (Stir Bar Sorptive Extraction) extraction method based on the Twister stir bar.

## Experimental

10 g carrot was grated into a common cooking shaker with 40 g pure water and then transferred together with a Twister (length 1 cm, phase thickness 0.5 mm) to a flask placed on a stirring plate set at about 700 rpm.

The solution was stirred for 60 minutes at room temperature (in accordance with standard analyte absorption on Twister) with adequate sealing of the container.

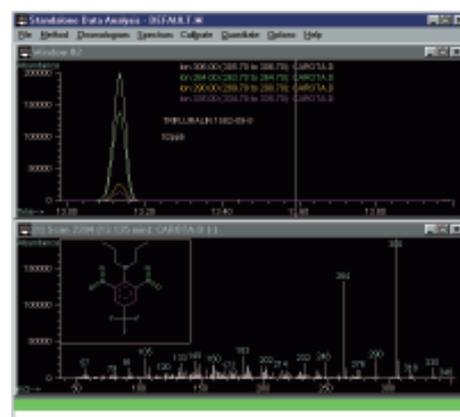
The Twister was washed in purified water, dried with absorbant paper and transferred into the Thermo Desorption System TDS 2, connected to the GC-MS, previously employed for the analysis with the classic method.

## Results

A number of volatile and semi-volatile components were extracted from the sample, constituting the aroma and perfume of the carrot.

Extracting the characteristic ions of the Trifluralin we detected its retention time and the spectrum was searched using the Agilent pesticide's spectra library. This gave a „match quality“ of 95 %, which increased to 97 % after the background subtraction.

The signal to noise ratio calculated on the analysis performed with the classic extraction gave a RMS result of almost 500/1 while the SBSE method exceeded 5000/1.



**Expansion in export department**

# Coordination of worldwide business

In the past few years, GERSTEL has widened its international activities. The company with its headquarters in Mülheim an der Ruhr, Germany, has two subsidiaries, GERSTEL Inc. in the USA and GERSTEL AG in Switzerland and is responsible for distribution in more than 30 countries throughout the world. This has led to an increase in the requirements for the company, and was reason enough to expand the export department.

**Sales**

Bernd Wiesend is an engineer and came to GERSTEL from the Federal Health Office Germany in 1992. He was in charge of the Berlin



**Jan Pieter Stoutjesdijk**

Office of the company for three years, and became Sales Manager for Germany in 1995. In 1999 he became responsible for developing the export business. Since September 2001, Bernd Wiesend is supported by Jan Pieter Stoutjesdijk, who hails from the Netherlands, and was a national sales representative from 1996 to 1998, before switching to our Dutch Distributor Analytical Application Brielle B.V. There he gained experience in export, which he can now use in working once more for GERSTEL to



**Bernd Wiesend**

enlarge the activities of the company, particularly in Europe, Africa and the Eastern.

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pieter\_stoutjesdijk@gerstel.com

**Service**

Bernd Wegmann has worked for GERSTEL for 15 years, and for the past five years he has been responsible for international service. He is now responsible for the technical support of distributors, and training and support for our instruments and systems, both in the headquarters in Mülheim an der Ruhr and also for distributors on the spot. Because of the marked increase in worldwide sales partners, the work has been becoming more and more complex, and more support was required. Thomas Albinus, a chemical engineer, now supports Bernd Wegmann. Since 1999, he has been acting as a service engineer for the company in Germany. In future, Thomas Albinus will be responsible for Europe and Africa.



**Bernd Wegmann**

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**Thomas Albinus**

**GERSTEL on the www:**

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**Imprint****Published by**

GERSTEL GmbH & Co. KG,  
Aktienstrasse 232 – 234,  
45473 Mülheim an der Ruhr  
Germany

**Editor**

Guido Deußing,  
ScienceCommunication,  
Neuss, Germany

ISSN 1619-0076

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**Design**

Paura Design, Hagen, Germany

**Printed by**

BasseDruck, Hagen, Germany

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**Agilent Technologies**  
Promoting the HP Way  
Premier Solution Partner  
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