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**NOTOX - Safety and Environmental Research**

## GERSTEL provides single source solution for instrumentation and service



Launching a new chemical or pharmaceutical product requires an enormous technical and organizational effort. Dr. Klaas Noorduyt, a toxicologist, spotted a niche market in this field, and founded the company NOTOX in the Netherlands in 1982.

With its 225 employees, NOTOX offers management and laboratory services to help its customers meet the global safety and environmental research requirements for new product development for the pharmaceutical, agrochemical and chemical industries. The company provides services needed to get a product registered in the countries in question. "Basically our customers need only focus on their production and their distribution channels", says Dr. Hans Stieltjes, head of the Bioanalytical Department, "NOTOX takes care of the rest".

The main task of the Bioanalytical Department at NOTOX is to determine the concentrations of medicinal drugs in blood, plasma and urine of subjects who take part in pre-clinical and clinical studies. NOTOX is a GLP accredited laboratory and is experienced in meeting FDA requirements for new drugs as well as EPA requirements for new chemicals. Dr. Stieltjes adds: "We help our customers to uncover costly errors - and make the necessary corrections at an early stage".

The bioanalytical department uses LC-MS instrumentation for method development and validation. Preference was given to SCIEX mass spectrometers and the Agilent Technologies

LC 1100 liquid chromatograph. But NOTOX also values solutions from a single source, which was not the case with the combination selected here. "We always needed two service technicians for maintenance of the system" Dr. Stieltjes said, and it appeared as though things were getting even more complicated. "What we were missing in our LC-MS system", he explains, "was a rapid and flexible auto-sampler that could handle both standard vials and 96 deep-well plates in a single run." And it needed to be a high-throughput sampler! The GERSTEL MultiPurpose Sampler (MPS 3) was taken into consideration. "But then we would have yet another supplier, which would bring us even further away from getting service and support from a single source."

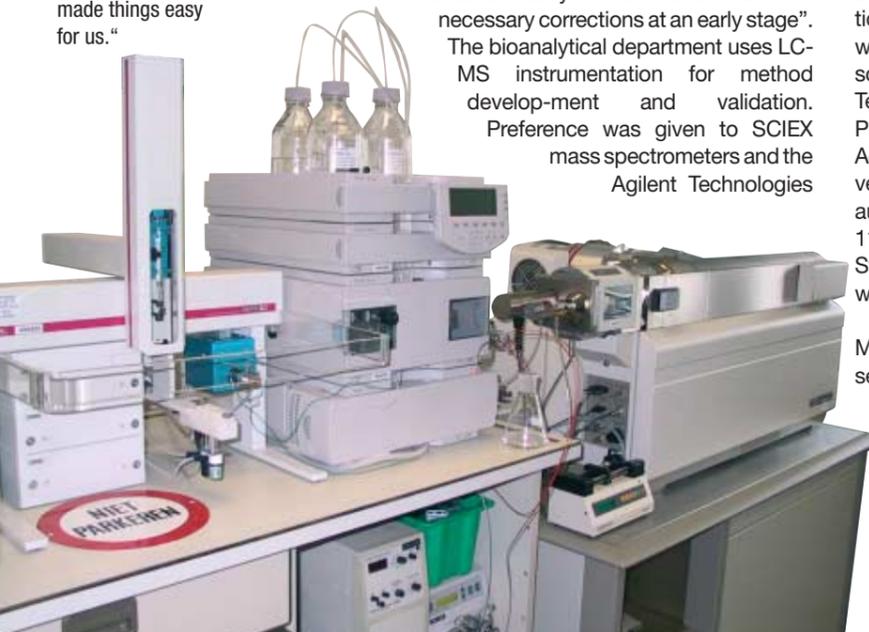
Dr. Stieltjes discussed the matter with Jan Pieter Stoutjesdijk, GERSTEL International Sales Representative who was able to provide the right solution: GERSTEL is an Agilent Technologies Premier Solutions Partner and is able to service Agilent systems, offering a single vendor solution for MPS 3 autosamplers and the Agilent 1100 LC system. This gave Dr. Stieltjes and NOTOX exactly what they wanted.

"We chose the GERSTEL MultiPurpose Sampler, and got service and support from a single source for the LC and MPS 3. SCIEX will continue to look after the MS. To avoid unnecessary downtime, we agreed that GERSTEL and SCIEX will coordinate their activities and visit us at the same time when we need them. We are happy to say that GERSTEL has made things easier for us" said Dr. Stieltjes. (Further information about NOTOX in the internet: [www.notox.nl](http://www.notox.nl))

**GERSTEL visit NOTOX**

"There was something missing in our LC-MS system."

**MPS 2 with a SCIEX MS and an Agilent Technologies LC 1100:** "GERSTEL made things easy for us."

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No. 4

September 2003

**Quality of tap and drinking water**

## The GERSTEL Twister sniffs out causes of bad odors



**Dr. Hans Stieltjes**  
with GERSTEL  
International Sales  
Representative Pieter  
Stoutjesdijk (left)

GERSTEL Headspace ChemSensor  
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Sensory Panels for  
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MultiPurpose Sampler (MPS 2)  
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productivity and  
flexibility for GC**



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# Drinking water has to be safe and reliable

The General Assembly of the United Nations (UN) has declared 2003 „International Year of Fresh Water“, while Europe and the USA are flying to Mars - partly to look for water. Pessimists and doomsayers might have you believe that this reflects our critical situation on planet earth. It is not quite that bad. Globally speaking, there is enough water. The difficulty lies in the distribution and quality of our available resources. Whereas Canada, Austria or Ireland, have more than enough water, there is too little in Australia, the Middle East and Northern China. The UN draws a dramatic picture in the World Water Report, presented in March 2003. According to the report, of the 9.3 billion people who will be living on earth by 2050, as many as seven billion will go thirsty.



The main problem is access to clean drinking water. Though it is the most important resource of all, clean drinking water is in short supply for about 1.1 billion people world-wide. According to the UN, 6,000 people die every day (the equivalent of about two million every year) due to unsanitary conditions and lack of access to clean, safe water.

## Water crisis in developing countries

Part of the problem is waste water. Untreated waste water from more than 2 billion people around the world winds up contaminating local sources of fresh water. It has been calculated that every liter of wastewater contaminates up to eight liters of fresh water. Not surprisingly, it is primarily people in developing countries who are facing these problems.

## Worldwide water challenges

While many developing countries are facing water shortages, industrialized countries are facing other challenges. Germany, for example, is listed as number 57 on the international water quality ranking list and is thus second-to-last in Europe. Fertilizers, pesticides, and various other man-made substances contaminate groundwater and surface water, i.e. the sources of

drinking water. In order to improve the safety of drinking water, the World Health Organisation (WHO) has developed guidelines for a number of substances and indicators for pathogens that can be found in water. Based on these guidelines, the European Union (EU) has specified concentration limits that have to be implemented in national legislation by member states. In Germany, new drinking water regulations have been in force since the beginning of this year, creating a basis for further improving the quality of the drinking water.

## Black box supply system: how safe is our drinking water really?

Item 4 of the Water Safety Plan in the 3rd edition of the „Guidelines for the quality of drinking water“ issued by the World Health Organisation (WHO) in 2003 contains the following text: „Detection of microbiological and chemical substances in water is generally a slow, complicated and expensive process“. This is a problem because pollutants that get in the water supply system can remain undetected since they can only be found through laboratory analysis.

The WHO suggests the establishment of early-warning systems involving more checks at more critical points in the supply system. The analytical technology and methods used, however, depend on many different national standards and regulations. Since these are generally not updated very frequently, they may lag behind the latest available technology.

For many years, GERSTEL has provided innovative solutions in the field of sample preparation and pre-concentration for GC and LC analysis. Two new automated sample preparation techniques have recently been introduced by GERSTEL, which could help to improve the quality of water analysis and thus ultimately the quality of our water supply.

## Membrane Extraction: Automated extraction of waste water and complex samples

Membrane Extraction is an innovative extraction process that enables direct liquid extraction of dirty effluents or emulsions. The technique was developed by the UFZ Environmental Research Centre, Leipzig-Halle, Germany and the product subsequently developed and

marketed by GERSTEL. The Membrane Extraction technique enables automated solvent extraction of liquid samples while keeping the liquid phases separated by a permeable membrane. It is now possible to perform liquid-liquid extractions no matter how undefined the phase separation is. Examples are samples with a high level of suspended solids, water-fat emulsions such as milk, or samples which contain detergents.

Preparing a sample for automated Membrane Extraction is very simple: The sample is placed in a vial after which an extraction membrane is inserted and the

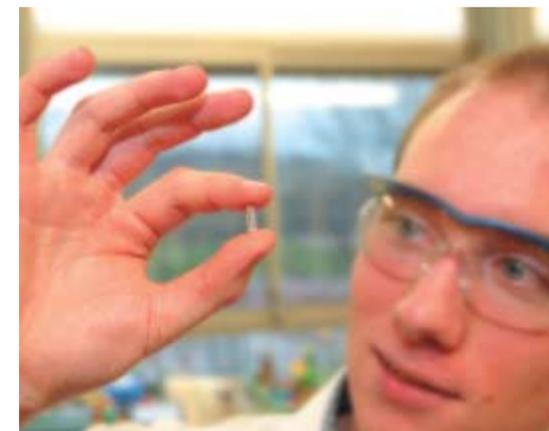
Figure 1 Schematic diagram of Membrane Extraction



vial is sealed. The rest of the analysis can be completely automated using the GERSTEL MultiPurpose Sampler (MPS). Solvent is added, the sample vial can be heated or agitated to improve extraction efficiency, and when the extraction is complete, the solvent can be injected into a GC or HPLC system. If pre-concentration is needed, the MPS autosampler can automatically perform a Large Volume Injection.

## Better drinking water thanks to GERSTEL Twister technology

The GERSTEL Twister is another promising new technology that offers improved and simplified sample preparation for determination of pollutants and off-odors in water. Journal publications and many customer applications have already shown the value of the Twister for easy water analysis with detection limits as low as sub-ng/L for pesticides and other semi volatile



## The GERSTEL Twister

is a magnetic stir bar, coated with a layer of polydimethylsiloxane (PDMS). While stirring at up to 2000 revolutions per minute, the Twister extracts organic compounds from the sample and concentrates these in the PDMS phase.

organic compounds in water (Leon et al., J. Chrom. A, 999 (2003) 91-101).

The Twister technology is also a powerful tool for identification of contaminants that cause off-odors, which can greatly influence consumer perception of water quality. An expert user of the technique in this field is David Benanou, laboratory manager and sensory expert from Veolia Water. The company is one of the biggest water suppliers in the world and was previously known as Vivendi Water. In one recent case, complaints were made about unpleasant water odour and taste at several locations in Sweden in the Veolia Water supply area (see also pages 4-7).

David Benanou was asked to investigate the matter on location in Sweden. After developing first impressions through sensory tests, Benanou used the revolutionary GERSTEL Twister to extract organic chemical compounds from the water for GC analysis.

## GERSTEL Twister: no extensive sample preparation is required

The Twister is a magnetic stir bar, coated with a layer of polydimethylsiloxane (PDMS). The Twister technique is also referred to as Stir Bar Sorptive Extraction or SBSE. The special twist: While stirring at up to 2000 revolutions per minute, the Twister extracts organic compounds from the sample and pre-concentrates these in the PDMS phase. The Twister is then removed, and the compounds are determined through the use of a GERSTEL thermal desorption system coupled with a GC/MSD. No extensive sample preparation is required.

Veolia Water tries to improve the quality of its drinking water in three phases: „We look first of all for the causes of the odor using Twister technology“ says David Benanou, „then we consider how off-odors develop, how they get into the water, and finally we take action to eliminate the cause or to reduce the concentration level. The Twister gives us excellent performance thanks to the simple handling and its extraordinary pre-concentration capability.“

David Benanou very quickly had results available and the causes of the off-odor were identified: minute amounts of geosmin and anisole, which were probably products of bacterial degradation. „What we found was comparable to one drop in enough water to fill ten Olympic-size swimming pools“, says Benanou.

Incidentally: shortly after the investigation in Sweden was completed, an inquiry came from Korea. Odor appears to be a factor spoiling the quality of tap water there as well and David Benanou is on his way. In his luggage: plenty of GERSTEL Twisters.

Yours sincerely,

Eberhard G. Gerstel



David Benanou  
Program Manager  
and Sensory Expert  
of Veolia Water  
formerly Vivendi  
Waters Laboratory

Twister goes  
Swedish Press  
because Benanou  
found geosmin  
and anisoles in tap  
water.



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**Quality of tap an drinking water**

# GERSTEL Twister sniffs out causes of bad odors

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**Introduction**

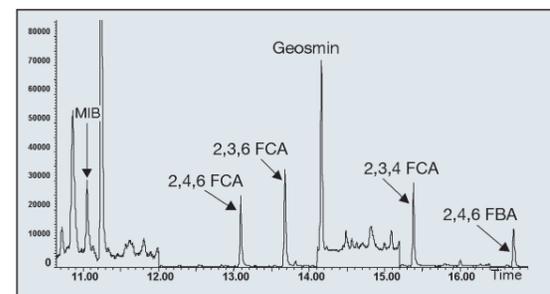
The presence of low levels of malodoros compounds in tap water can greatly influence the consumer's perception of the quality of the water. Most of the compounds present produce chlorine-like, earthy and musty odors. Although the compounds that produce the odors are present at harmless levels, the disagreeable smell gives the consumer doubts about drinking the water.

The target of our work was to develop a procedure to quickly and reliably analyze six organic odor compounds in water. The six were: Geosmin, 2-methylisoborneol, 2,4,6-trichloroanisole, 2,3,6-trichloroanisole, 2,3,4-trichloroanisole and 2,4,6-tribromoanisole.

Quantitation at the sub-nanogram level was needed. This represents detection levels at or below the compound's odor threshold level (Tab. 1). We used gas chromatography/mass spectroscopy (GC/MS) as the analytical instrumental technique and the GERSTEL Twister, or Stir Bar Sorptive Extraction (SBSE), for sampling and sample preparation. Compounds were thermally released from the Twister stir bar using a GERSTEL Thermal Desorption System (TDS).

**Results and discussion****Influence of extraction time**

The kinetics of sorption of the six components into the PDMS coating of the Twister were examined. Spring water, spiked with 2 ng/L of each compound (Fig. 1), was extracted for different lengths of time in the 15 to 300



**Figure 1:** SIM chromatogram of spring water spiked with 2 ng/L of each component.

minute range. For each compound, sorption occurred relatively quickly for 120 minutes, and then slowed without reaching a plateau. An extraction time of 120 minutes was empirically chosen for routine analyses with high sample throughput.

**Influence of the sample volume**

Maximum recoveries can be calculated from octanol-water distribution coefficients ( $K_{ow}$ ) using the KOWWIN software (SRC, 2000). Table 2 shows the experimentally determined and calculated log  $K_{ow}$  values for each compound. For the experiment, different volumes of spring water (10 to 200 mL) were spiked with 1 ng of each compound and extracted for 2 hours with the Twister (20 mm, 47  $\mu$ L PDMS).

The experimental results were in agreement with theory – the larger the sample volume, the lower the

**Table 2:** Octanol-water distribution coefficient ( $K_{ow}$ ) of the compounds analyzed

Name	experimental log $K_{ow}$	Calculated log $K_{ow}$
2-Methylisoborneol	3.31	2.85
2,4,6-Trichloroanisole	3.85	4.01
2,3,6-Trichloroanisole	3.64	4.01
Geosmin	n/a	3.57
2,3,4-Trichloroanisole	3.74	4.01
2,4,6-Tribromoanisole	4.48	4.75

recovery – but were below the anticipated values. Even after stirring for two hours, equilibrium had not been reached. The difference between experimental and anticipated values increased with increasing sample volume, depending on the particular compound.

The amount of compound concentrated in the PDMS coating increased with sample volume. For most compounds there was an increase up to 100 mL sample volume; increasing the sample volume to 200 mL brought no significant gain in response. To measure concentrations at the odor threshold level for each compound, two aliquots of 100 mL were extracted in parallel, each with a separate Twister. Both Twisters were subsequently desorbed at the same time.

**Influence of storage after extraction**

Six samples of spring water spiked with 2 ng/L of each compound were extracted. 10 mL of each sample was extracted with a Twister for two hours. One Twister was immediately desorbed, the other five were stored in vials at 4°C for later analysis.

Result: Even after storage for one week no loss of compounds was seen from the Twisters. This allows the conclusion to be drawn that when chromatographic analysis cannot be performed immediately, it is better to extract and then store the Twister than to store the original sample. When complaints are received about off-odors or bad taste of water, the compounds causing the problem should promptly be extracted and trapped. Water samples themselves need not be sent to a laboratory, however, as extractions can be made on the spot by the customer.

Name	Abbreviation	Taste	Odor threshold	CAS Number
2-Methylisoborneol	MIB	earthy	5 - 10 ng/L	n/a
2,4,6-Trichloroanisole	2,4,6-TCA	musty	0.1 - 2 ng/L	6130-75-2
2,3,6-Trichloroanisole	2,3,6-TCA	musty	0.2 - 2 ng/L	50375-10-5
Geosmin	Geosmin	camphor-like	1 - 10 ng/L	19700-21-1
2,3,4-Trichloroanisole	2,3,4-TCA	musty	0.2 - 2 ng/L	54135-80-7
2,4,6-Tribromoanisole	2,4,6-TBA	musty	0.15 - 10 ng/L	607-99-8

**Table 1:** Odor components determined

## Equipment used and analytical conditions

**Gas chromatograph 6890 (Agilent Technologies)**

**Column:** HP5-MS, length 30 m, i.d. 0.25 mm, film thickness 0.25  $\mu$ m

**Carrier gas:** Helium

**Flow:** 1.5 mL/min (constant)

**Temperature profile:** 50 °C – 2 min – 10 °C/min – 200 °C – 25 °C/min – 300 °C (2 min)

**Mass spectrometer 5973 (Agilent Technologies)**

**Mode:** Single-Ion-Monitoring

**Thermal Desorption System (TDS A) (GERSTEL)**

**Mode:** Split

**Temperature program:** 30 °C (0.8 min) – 60 °C/min – 280 °C (5 min)

**Cooled Injection System (CIS 4) (GERSTEL)**

Cryofocusing at -100 °C. Subsequent heating at 10 °C/s to 300°C, holding 2 minutes. Injection is made with solvent venting.

**Twister (GERSTEL)**

20 mm, 0.5 mm PDMS

**Chemical standards and reagents**

- Methanol (pesticide quality, Merck, Darmstadt)
- Spring water for blanks and standards
- 2-methylisoborneol, 2,4,6-trichloroanisole, 2,3,6-trichloroanisole, 2,3,4-trichloroanisole, 2,3,6-tribromoanisole, geosmin and 2,4,6-trichloroanisole D5 (Promochem, France)
- Stock solution, consisting of spring water and 1  $\mu$ g/L each of MIB, geosmin and the haloanisoles. Stable for 1 month at 4°C.
- Internal standard: 2,4,6-TCA D5 in spring water (20  $\mu$ g/L). Stable for 1 month at 4°C.

**Extraction**

Extractions of analytes done in parallel: 100 mL water sample, 5 mL methanol, 40  $\mu$ L internal standard and a Twister were placed into a 125 mL volumetric flask. The water sample was stirred for two hours at room temperature. The Twister was removed, patted dry, transferred into a glass desorption tube and desorbed in the TDS.



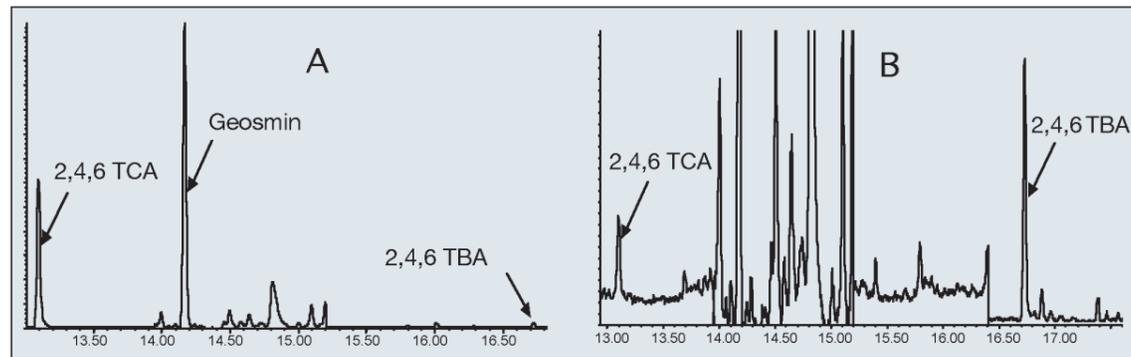


Figure 2: Chromatograms obtained for samples A and B in SIM-mode (case 1)

### Validation of the method

The method was validated according to Guidelines XP T 90-210 of AFNOR, the French Institute for Standardization and member of the ISO; the validation criteria were fulfilled for all target compounds (Tab. 3). Practical tests were made using real water samples that had been analyzed after complaints of bad taste and odour.

### Case 1

Two samples (A and B) were taken in the household of a customer: Sample A had a pronounced musty smell, sample B a somewhat musty but pronounced metallic smell. Extraction was carried out with the Twister, the determination of MIB, geosmin and haloanisoles was performed using GC/MS in SIM-mode. Table 4 shows the quantitative results, figure 2 the chromatograms.

Table 3: Scan chromatogram of sample A (case 1)

	R	LOQ ng/L	Repeatability %	Trueness %	Reproducibility %
MIB	0.9987	1	4-10	89	13
2,4,6-TCA	0.9998	0.1	1-5	97	4
2,3,6-TCA	0.9998	0.1	4-11	97	5
Geosmin	0.9991	0.5	2-10	83	9
2,3,4-TCA	0.9998	0.2	7-15	87	13
2,4,6-TCA	1.0000	0.2	2-9	91	15

The compound concentrations found in the samples explain the musty smell. To identify further compounds which could cause the off-odor, the samples were again extracted with the Twister, this time without internal standards, and analyzed using GC/MS in SCAN-mode.

The olfactory detection of sample A gave a pronounced musty smell at the retention times for 2,4,6-TCA and geosmin; also obvious was a typical medicinal smell at 8 minutes, and a smell of solvent at 14 minutes. The olfactory detection of the B sample gave a medium musty smell at the retention time for 2,4,6-TBA as well as a typical medicinal smell at about 8 minutes.

The mass spectrum and isotope relationships of sample A showed a brominated component after 8.4 minutes and a chlorinated component after 13.9 minutes. The medicinal smell could be attributed to dibromomethyl iodide, a chlorinated by-product, the smell of solvent to tetrachlorobenzene (Fig. 3). Dibromomethyl iodide was also shown to be present in sample B.

Table 4: Concentration of the target components in sample A and B

	Sample A[C] (ng/L)	Sample B[C] (ng/L)
2-Methylisoborneol	< 1	< 1
2,4,6-Trichloranisole	8.9	0.2
2,3,6-Trichloranisole	< 0.1	< 0.1
Geosmin	5.2	< 0.5
2,3,4-Trichloranisole	< 0.2	< 0.2
2,4,6-Tribromanisole	0.4	1.3

### Case 2

Water from a tank near Paris had an off-odor. The reason was unknown. During sampling, cracks in the tank were noticed, and taste analysis of the water taken indicated a chlorinated taste, overlaid with an intense musty taste (threshold test No. 5). But what caused this drinking water, which was sourced from ground water, to have such an intense off-odor? Prior to being stored in the tank as drinking water, the ground water was treated as follows:

It was aerated and filtered through sand to remove iron, then chlorinated at the tank inlet to kill bacteria. The coating of the tank was impermeable to water, consisting of synthetic cement produced by mixing a grey, elastic cement with a white synthetic resin in aqueous solution. The coating was very elastic, but released no organic compounds. The filtered and chlorinated water was extracted with the Twister and quantitatively analyzed to determine the previously mentioned compounds.

Table 5 shows the results. The only one of the six taste compounds found in the chlorinated water was 2,4,6-tribromoanisole at a concentration of 5.6 ng/L. This explained the musty taste of the water; the filtered water appeared not to contain any of the six target compounds known to cause off-odor.

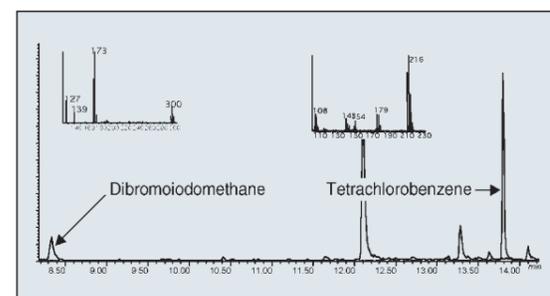


Figure 3: Scan chromatogram of sample A (case 1)

Olfactory detection of the filtered water did not bring any characteristic odor to the fore. Analysis of the chlorinated water, however, brought forward a very musty odour at the retention time of 2,4,6-TBA as well as various phenolic odors at 8, 14 and 17 minutes.

In order to analyze the phenolic components by gas chromatography, they were derivatized in a 10 mL water sample with 1 g K<sub>2</sub>CO<sub>3</sub> and 500 µL of acetic anhydride; GC/MS detection was performed in SCAN-mode. This procedure enabled us to determine that the sample contained 2,4,6-trichlorophenol and 2,4,6-tribromophenol alongside phenol. The result of the sniff-test and MS detection are summarized in Table 6. Figure 4 shows the chromatograms obtained.

On the basis of these results, the assumption was made that the tank coating had released phenol, which reacted with excess chlorine and free bromide to 2,4,6-TCP and 2,4,6-TBP. In addition, 2,4,6-TBA may well have been synthesized by organisms that had settled on the surface of the coating. No answer was given as to why only 2,4,6-TBA was formed, despite the presence of 2,4,6-TCP and 2,4,6-TBP.

### Case 3

In this case it was evident that the sensory water quality got worse along the municipal drinking water pipeline. Complaints came from consumers living far away from the waterworks. Two samples were taken: at the outlet from the waterworks (A), the second in the house of a consumer at the end of the pipe system (B). Sample A had a chlorinated odor, whereas sample B smelled musty, marshy and earthy (threshold test: > 10).

Measurement gave no contamination of sample A with geosmin, MIB or haloanisoles. In sample B, however, 2,4,6-TCA and 2,3,4-TCA were found in concentrations of 0.1 ng/L and 0.2 ng/L respectively; but this did not explain the taste and odor. The water samples were again extracted with the Twister, but this time without internal standards, and then analyzed by GC/MS with olfactory and SCAN-mode detection.

The olfactory examination of sample B gave several odours, whereas the olfactory examination of sample A was negative. The results of the sniff-test and MS analysis are given in Table 7. Seven different odours could be detected by sniffing, of which some were in agreement with the odor profile analysis.

### Summary

A rapid SBSE-GC-MS-Olfactory method was developed for the determination of MIB, geosmin and haloanisole components in water.

The combination of GC/MS and the Twister (SBSE) led to very low detection limits for all components, near or below the odor threshold. The influence of extraction time, sample volume and storage time were examined, to improve the sensitivity of the measurement. The final method was validated according to AFNOR-Guidelines.

The linearity was examined with the correlation co-efficient (R) in the range from 0.9987 to 1.000. Repeatability and reproducibility were both below 15 percent and the recovery was between 87 and 117 percent depending on the component. After extraction with a Twister, the Twister could be stored for seven days under suitable conditions without any loss of analyte.

Table 6: Odors detected during the analysis of sample B (case 2)

Retention time (min)	Odor	Intensity	Qualification (acetate derivative)
8.5	phenolic	++++	Phenol
13.7	phenolic	++	2,4,6-Trichlorophenol
15.9	musty	+++	2,4,6-Tribromanisole
16.8	phenolic	+++	2,4,6-Tribromophenol

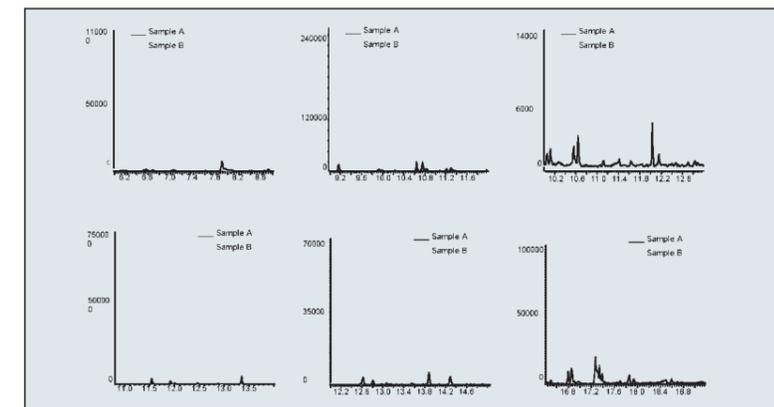


Figure 4: Comparison of the reconstructed chromatograms (retention indices, RIC) for each component smelled for samples A and B

When used for genuine, odor-loaded water samples, Stir Bar Sorptive Extraction (SBSE) provided good correlation between the odor profile analysis, the MS analysis and olfactory detection. SBSE was found to be a highly efficient and useful technique for the analysis of MIB, geosmin and haloanisoles.

### Conclusion

The procedure described in this paper provides a means of identifying odorous compounds in water at very low concentration levels. The determination can be performed much faster than was previously possible using traditional techniques.

Table 5: Concentration of the target compounds in filtered and chlorinated water (case 2)

	Filtered water	Chlorinated water [C] (ng/L)
2-Methylisoborneol	< 1	< 1
2,4,6-Trichloranisole	< 0.1	< 0.1
2,3,6-Trichloranisole	< 0.1	< 0.1
Geosmin	< 0.5	< 0.5
2,3,4-Trichloranisole	< 0.2	< 0.2
2,4,6-Tribromanisole	< 0.2	5.6

Table 7: Odors detected during the examination of sample B (case 3)

Retention time	Odor	Compound
7	sweat	Phenylacetaldehyde
7.8	marshy	Dimethyltrisulfide
10.7	lemony	Decanal ?
12.8	sweat	not identifiable
12.9 to 15.2	musty	Alkylbromobenzene isomer
16.07	rancid	Isopropyl dodecanoate ?
16.8 to 17.4	tar	Diisopropyl naphthalene
20.15	tar	Dodecahydrophenanthrene

# Headspace Analysis of Volatile Contaminants in Water

Volatile contaminants in waste or waste water from industry can pose a threat to aquatic systems. Examples are the use of chlorinated solvents for cleaning purposes, the accidental release of fuel compounds and the contamination of water by substances released from contaminated industrial sites.

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Monitoring of these compounds is required at µg/L quantities for the protection of human health and aquatic ecosystems. As releases of these compounds are almost impossible to remediate, it is of great importance to investigate rising trends in environmental concentrations well before critical concentrations are reached.

A headspace gas chromatography mass spectrometry system has been set-up in order to determine volatile compounds in water. After equilibration at elevated temperature a sample from the headspace is injected into a GC with Cooled Injection System (CIS). The mass spectrometric detection allows identification of contaminants and the isotope dilution quantification with deuterated or C<sub>13</sub> internal standards. The system is highly automated and reduces the risk of cross-contamination to a minimum. The Headspace-GC/MS consists of an Agilent Technologies 6890 gas chromatograph with 5973N mass spectrometer, two GERSTEL CIS injection systems, a GERSTEL MultiPurpose Sampler (MPS 2) and a GERSTEL Thermal Desorption System (TDS A).

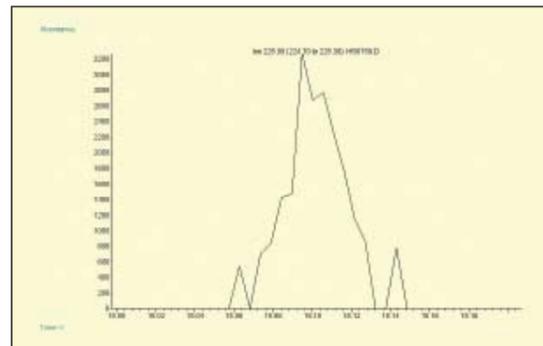
**Table 1:** Volatile compounds which were examined with headspace gas chromatography and detected with mass spectrometry.

Compounds	QS for In-Tr waters (WFD)*	LoD-HS-SIM	LoQ-HS-SIM
Dichloromethane	8.2 µg/L	0.010 µg/L	0.050 µg/L
Trichloromethane	3.85 µg/L	0.100 µg/L	0.250 µg/L
Carbon tetrachloride	7.2 µg/L	0.500 µg/L	1 µg/L
Benzene	16a µg/L	0.100 µg/L	0.200 µg/L
Trichloroethylene	10 µg/L	0.002 µg/L	0.005 µg/L
Tetrachloroethylene	10 µg/L	0.001 µg/L	0.005 µg/L
1,2,4 Trichlorobenzene	1.8 µg/L	0.005 µg/L	0.010 µg/L
1,2,3 Trichlorobenzene		0.005 µg/L	0.010 µg/L
Naphthalene	2.4 µg/L	0.001 µg/L	0.005 µg/L
Hexachlorobutadiene	0.003 µg/L	0.002 µg/L	0.005 µg/L
1,2 Dichloroethane	1060 µg/L	0.500 µg/L	1 µg/L

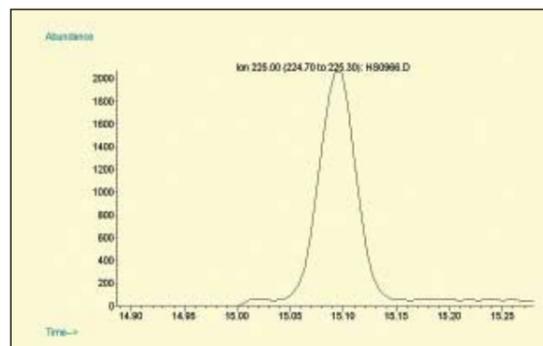
\* Quality standard referring to the annual average concentration for inland and transitional waters as proposed by the final outcome of the study: "Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive", Lepper P. (2002), Fraunhofer-Institute Molecular Biology and Applied Ecology

The method meets required performance criteria for drinking water analysis and allows even much lower detection, down to few ng/L for analysis of concentration trends. The method can be applied to a minimum concentration of 0.1 µg/L in SCAN-mode (compound dependent) allowing target and non-target analysis while for target analysis in SIM-mode (single ion monitoring) the method was successfully tested with a minimum concentration of 0.005 µg/L (compound dependent).

**Figure 1:** 50 ng/L hexachlorobutadiene measured in SCAN-mode. Ion 225 is used to quantitate also in sim mode (Figure 2).

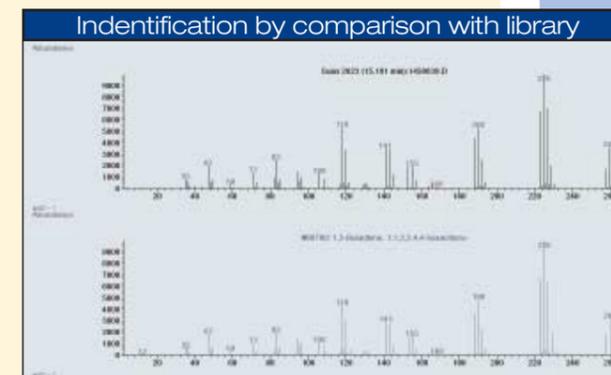
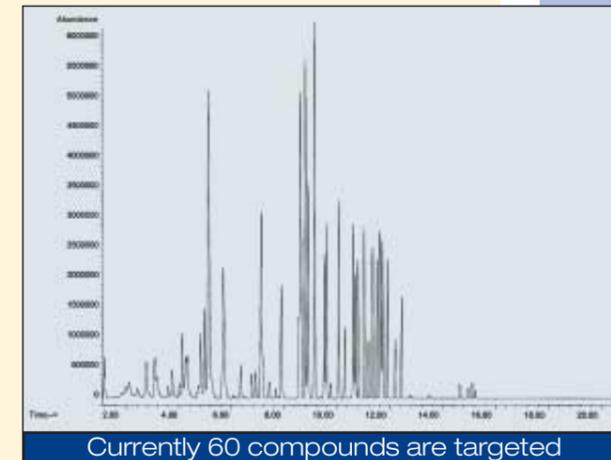


**Figure 2:** 50 ng/L hexachlorobutadiene measured in SIM-mode. It is evident that peaks are better defined and sharper.



## Analysis of 60 volatile compounds with headspace GC / MS

- 1) ?
- 2) Dichlorofluoromethane
- 3) Chloromethane
- 4) Vinyl chloride
- 5) Bromomethane
- 6) Chloroethane
- 7) Trichlorofluoromethane
- 8) Bromodichloromethane
- 9) cis - 1,2 - Dichloroethylene
- 10) t rans - 1,2 - Dichloroethylene
- 11) Methylene chloride
- 12) 1,1 - Dichloroethylene
- 13) tert -Butylmethylether
- 14) 1,1 - Dichloroethane
- 15) 2,2 - Dichloropropane
- 16) Chloroform
- 17) 1,1 - Dichloropropylene
- 18) 1,2 - Dichloroethane
- 19) Trichloroethylene
- 20) Bromochloromethane
- 21) 1,1,1 - Trichloroethane
- 22) Carbon tetrachloride
- 23) 1,2 - Dichloropropane
- 24) Dibromomethane
- 25) Benzene
- 26) Toluene
- 28) Tetrachloroethylene
- 29) Bromoform
- 30) Chlorobenzene
- 31) Styrene
- 32) p-Xylene
- 33) o-Xylene
- 35) 1,2 - Dibromomethane
- 36) 1,3 - Dichloropropane
- 37) 1,1,2 - Trichloroethane
- 38) t rans - 1,3 - Dichloropropylene
- 39) cis - 1,3 - Dichloropropylene
- 40) 1,1,1,2 - Tetrachloroethane
- 41) 1,1,2,2 - Tetrachloroethane
- 42) Ethylbenzene+m-Xylene
- 43) Dibromochloromethane
- 44) 1,2,3 - Trichloropropane
- 46) Isopropylbenzene
- 47) n-Propylbenzene
- 48) 2-Chlorotoluene
- 49) 4,-Chlorotoluene
- 50) tert -Butylbenzene
- 51) sec-Butylbenzene
- 52) 1,3-Dichlorobenzene
- 53) 1,4-Dichlorobenzene
- 54) 1,2-Dichlorobenzene
- 55) Bromobenzene
- 56) 1,3,5-Trimethylbenzene
- 57) 1,2,4-Trimethylbenzene
- 58) p-Isopropyltoluene
- 59) n-Butylbenzene
- 60) 1,2,4-Trichlorobenzene
- 61) Naphthalene
- 62) 1,2,3-Trichlorobenzene
- 63) 1,2-Dibromo-3-chloropropane
- 64) Hexachlorobutadiene



## Instrument parameters

**MultiPurpose Sampler (MPS 2) (GERSTEL, autosampler)**  
 Sample volume 1.5 mL  
 Incubation temperature 60 °C  
 Incubation time 20.00 min  
 Syringe temp. 70 °C

**Cooled Injection System (CIS 4 PLUS) (GERSTEL)**  
 Equilibration time 0.2 min  
 Initial temperature - 40 °C  
 Initial time 0.15 min  
 Rate 12 C / min  
 Final temperature 200 °C  
 Final time 3 min

**5973 GC / MSD: HS / GC (GC 6890 Series, Agilent Technologies)**  
 Iso time SB: 0 min  
 Iso temperature SB: 40 °C  
 Iso time 1: 10 min  
 Rate: 8 °C / min  
 Iso temperature 2: 200 °C  
 Iso time 2: 5 min  
 Zone temperature transfer line 230 °C  
 Capillary column: DB-VRX (J&W)  
 Column length: 30 m  
 Column i.d.: 0.32 mm  
 Film thickness: 1.8 µm  
 Glass vaporization tube filled with Tenax TA  
**HP 5973 GC / MSD: MSD 5973**  
 Mass range 35 – 500  
 Solvent delay 1.00 min  
 Zone temperature MS Source 230 °C  
 Zone temperature Quad 150 °C

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GERSTEL is represented in more than 40 countries world-wide by our own sales and support organization and by a network of distributors. Our distributors are carefully selected according to their experience with analytical instrumentation and their ability to represent and support GERSTEL modules and solutions. Support is a critical factor in offering the best customer value as part of the overall solution. Our distributors can rely on the GERSTEL International Service Support at all times. Only recently, the list of countries with GERSTEL distributors has been extended to include **Egypt, Bahrain, Kuwait, Oman and Qatar**. For contact details, please see the distributor list in this magazine.

In order to provide the best possible support for our many customers in **The Netherlands**, GERSTEL products will be represented exclusively by *Da Vinci*

*Europe BV* as of October 1, 2003. Centrally located in Schiedam, the Netherlands, *Da Vinci Europe BV* offers extensive experience in selling and supporting analytical instruments and in servicing Agilent products.

We are sorry to report the loss of our friend and long-time representative in **Poland**, Mr. Marek Daniewski Ph.D., from the company *Chromtec*. Our condolences and best wishes go out to Marek's family.

The new GERSTEL distributor in Poland is the company *Perlan Technologies Polska Sp. z o.o.* based in Warsaw. *Perlan Technologies* was formed from the former Agilent Technologies organization in Poland and is an authorized Agilent Technologies distributor and service agent. We are certain that *Perlan Technologies* will provide outstanding support to the Polish GERSTEL customers.

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## MPS 2 User benefits

Whichever sample preparation or injection technique you use, you will enjoy a key benefit of the GERSTEL MultiPurpose Sampler (MPS 2): Complete and convenient control of this versatile sampler through the GERSTEL MASTer Software. The MASTer Software is completely integrated in the Agilent ChemStation software. In other words, GC and MPS 2 are controlled by a single software user interface.



### GERSTEL MultiPurpose Sampler (MPS 2)

# Enhanced productivity and flexibility for gas chromatography

**The GERSTEL MultiPurpose Sampler (MPS 2) is more than just a widely used and highly productive autosampler. While several companies offer autosamplers for GC, the GERSTEL MPS 2 stands apart from all the rest. It offers more capabilities for introducing samples into the GC instrument than any other autosampler, providing unparalleled versatility, ease-of-use, and productivity to the analytical laboratory. The MPS 2 can be configured to meet demanding analysis requirements for both routine analysis and for leading-edge research. The MPS 2 is a proven autosampler for a wide range of applications, including industrial quality control, forensics investigation, flavor and fragrance profiling and environmental analysis.**

The MPS 2 can be configured to meet individual requirements. The sampler is compatible with most current gas chromatographs. Depending on the configuration, the MPS 2 performs standard liquid injection, large-volume liquid injection, headspace injection, solid phase micro-extraction (SPME) fiber sampling and injection, and fully automated desorption of GERSTEL Twister Stir Bars used for Stir Bar Sorptive Extraction (SBSE).

In order to use the MPS 2 for Large Volume Injection (LVI), a GERSTEL Cooled Injection System (CIS) is required. A special LVI-calculator for rapid method development is provided free of charge with the control software (GERSTEL MASTer Software) to facilitate this

analysis. In any configuration, the MPS 2 sampler can be conveniently operated. All injection steps are programmed from the same computer that controls the GC, or from the hand-held controller. These steps include syringe preparation, sampling, injection speed, solvent effects, rinse cycles, and standard addition.

Modular accessories allow the MPS 2 to be upgraded to a multifunctional sample preparation system for gas chromatography. Up to three trays can be mounted on the MPS 2. Up to 600 1-mL vials, up to 296 2-mL vials, and up to 96 Headspace vials can be set up for automated analysis. Sample trays can easily be exchanged, and these can be fitted with heating or cooling options to ensure optimal conditions for the samples.

Several versions of the MPS 2 are available for performing a wide variety of analytical tasks:

#### MPS 2 for Liquid injection

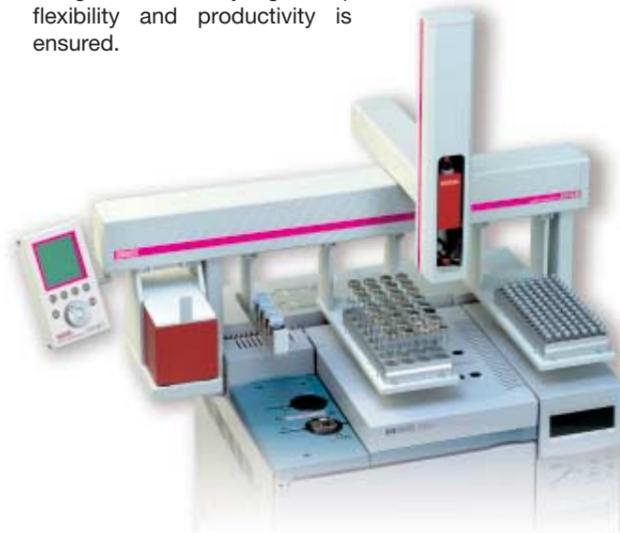
High productivity autosampler for liquid injection and large volume injection (LVI). The MPS 2 can be upgraded with Headspace, SPME, and the GERSTEL Twister Desorption Unit (TDU) options.

#### MPS 2L

Dedicated high productivity autosampler for liquid injection and large volume injection (LVI). The MPS 2L is a cost-effective version that can be upgraded to perform automated Twister (SBSE) desorption and analysis in combination with a TDU and GERSTEL Cooled Injection System (CIS).

#### Headspace Sampling

Headspace sampling capability can be added to the MPS 2 for automated, routine analysis of volatile compounds in solid or liquid samples. If liquid sampling is required, the change-over takes only a few seconds using a click-on syringe adaptor. Maximum flexibility and productivity is ensured.



**High Productivity** autosampler for liquid injection and Large Volume Injection: MPS 2

For temperature sensitive samples, both the trays and the agitator can be cooled using optional cooling accessories. Analyte preconcentration from large volume headspace injections – or from multiple injections – can be performed using a GERSTEL CIS Injector. Pre-concentration is typically used for applications such as halogenated hydrocarbons or BTX in water. Even when using a GC-FID system, the detection limit for benzene required by the new German Drinking Water Regulations (TWO) can directly be achieved.

#### SPME sampling

Due to the many benefits offered by Solid Phase Micro Extraction (SPME), this effective and convenient preconcentration technique has become widely used for many applications. The MPS 2 offers complete automation of SPME, including automated thermal equilibration and agitation of the sample, flexible height adjustment for liquid or gas phase sampling, and a separate bake-out station for automated reconditioning of the fiber between analyses.

#### The GERSTEL Twister Option

Any version of the MPS 2 can be upgraded for automated desorption of GERSTEL Twister stir bars. One Twister Tray holds up to 98 samples in individual sealed compartments for automated analysis. The Twister is a coated stir bar, used to extract organic compounds from aqueous or other polar liquid samples. The technique, known as Stir Bar Sorptive Extraction (SBSE), allows highly efficient extraction from a 10-20 mL liquid sample volume. When the Twister is desorbed in a Twister Desorption Unit almost 100 % transfer efficiency to the GC column can be achieved, enabling ultra-trace analysis of organic compounds. For this highly sensitive and productive analysis technique, GERSTEL provides the complete system, including a multiple-position magnetic stirring plate, the MPS 2 autosampler, and the TDU along with the well-proven Cooled Injection System.

#### MPS 2 Integrated ease-of-use:

No matter which sample preparation or injection technique you use, you will enjoy a key benefit of the GERSTEL MultiPurpose Sampler MPS 2: complete and convenient control of this versatile autosampler through the GERSTEL MASTer Software. When the MPS 2 is installed onto an Agilent Technologies GC instrument, the GERSTEL MASTer Software is fully integrated into the ChemStation software (Agilent Technologies).

For other manufacturers' GC instruments, the MASTer software works harmoniously and seamlessly alongside the GC software operating system.

#### Note of the Publisher

*We are very sorry that a misunderstanding occurred in our 2002 issue. We want to clarify that ABreg s.r.l. represented GERSTEL GmbH & Co. KG at the Milan Exhibition in October 2001 and has never changed its company name. ABreg is an existing and active company. Our co-operation with ABreg s.r.l. however was terminated in June 2002. Since then the GERSTEL distributor for Italy is: A.I.Tech s.r.l., C. so IV Novembre 58, 15100 Alessandria, Italy, Phone 0039 131 - 32 55 28, Fax 0039 131 - 25 78 47, e-mail ai.tech@libero.it. We sincerely apologise for any confusion which we may have caused.*

*The Publisher*

### Leading chromatography supplier

## Matriks AS - distributor of GERSTEL products in Norway



**The Matriks Team** (from left to right): Anette Johansen, Ørjan Espeseth, Anne Mørch (back row), Norunn Følsvik, Bo Fritzell (back row), Sølvi Holmefjord, Geir Skagestad (back row), Lene Camilla Vold.

»Oil-in-water-analysis«

In June 2002 Agilent Technologies ceased to have direct representation in Norway. The company Matriks A/S became the exclusive sales and support channel for Agilent Technologies. Founded by three former Agilent employees, Matriks went on to hire the entire experienced and competent staff from Agilent Technologies in Norway in order to ensure success. The market demands total solutions and Matriks has been building up their product portfolio and skills during the first year in business in order to serve the Norwegian market in the best possible way. Matriks is today the leading chromatography supplier in Norway, offering solutions, instruments and services to pharmaceutical, environmental, chemical and biochemical industries.

#### The Matriks team

The Matriks team is a group of dedicated young people. The members have extensive experience and competence in chemical analysis and analytical instruments, most of them previously worked for Agilent in Norway. As the business has grown, Matriks has hired additional new talent. The goal is to offer the best solutions and services to our customers through continuous development of the team.

#### The Matriks vision

The vision is to make Matriks the preferred supplier for businesses within chemical and biochemical analysis by offering high quality products, solutions and services to meet the customer's requirements.

GERSTEL GmbH & Co. KG is proud to have Matriks as our sole distributor in Norway. Close cooperation between GERSTEL and Matriks ensures that customers in Norway can get the full benefits of GERSTEL solutions.



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## GERSTEL Headspace ChemSensor

# As good as a Sensory Panel for Rating Carpets



Figure 1:

The GUT seal of quality Carpets were first granted the GUT seal in 1990; The word "GUT" means "Good" in German, but the abbreviation stands for „Gemeinschaft umweltfreundlicher Teppichboden“ (Association for Environmentally Friendly Carpeting). Carpet materials with the GUT seal of approval distinguish themselves by having less of the typical "new carpet" smell and by containing less than certain specified amounts of various pollutants (www.gut-ev.de).

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### Introduction

Most people in the industrialized world spend between 75 and 90 % of their time indoors. Our well-being is therefore directly influenced by emissions from the materials surrounding us such as building materials, household products, upholstery and carpet materials. In Germany, 80 % of all consumer complaints about new carpets are related to annoying odors.

The source of these odors could lie in the various raw materials used, or in additives used for the final finishing treatment. Chemical reactions which take place during the production of the carpet materials could also generate odorous compounds. Numerous substances including styrene, 4-phenylcyclohexene (4-PCH), aromatic hydrocarbons, alcohols and alkenes contribute to carpet odors<sup>1, 2, 3</sup>.

Although a correlation has not yet been proven between physiological problems and odor exposure, it is generally accepted that unwanted odors reduce the quality of life and can cause psychological distress<sup>4</sup>.

Until now, odors have mainly been sniffed out and identified using olfactory panels, which give hedonic ratings, indicating whether smelling a product is a pleasant experience or not. In such a process, only the perception of the odor and its intensity are taken into account. The procedure is based on Swiss Standard Method SNV 195651 for the determination of the odor impact of textiles<sup>5</sup> slightly modified to be used for carpets.

In practice, many odor analyses can be performed quickly, reproducibly and objectively with a chemical sensor system. The GERSTEL ChemSensor system, which is used for the work presented in this article, fulfills the criteria of the Association for Environmentally Friendly Fitted Carpets (GUT) (Fig. 1).

### A carpet can release three types of odors:

- 1. New carpet odor** Is set free within the first few days after being laid. Cannot be completely eliminated. Disappears from the room air after some time.
- 2. Additional odor** Intense and long-lasting. Perceptible even months after the carpet is laid. Overlaps the „new carpet“ odor.
- 3. Absorbed odor** Caused by odorant contaminants that are absorbed during storage or use of the carpet and released over time."

### Methods

#### Sensory panel

The analysis is performed using a sample of 120 cm<sup>2</sup>, which has been conditioned for 15 hours in a closed 2 L beaker at 37 °C and 50 % relative humidity (Fig. 2). These conditions represent an average living environment with floor heating or with exposure to direct sunlight. In time intervals of 15 minutes or higher, seven trained and experienced panel members sequentially evaluate the odor of the carpet. Each member then gives an individual rating of the experienced odor impression according to the following scale:

- 1 Odorless (no detectable odor)**
- 2 Limited odor**
- 3 Tolerable odor**
- 4 Annoying odor**
- 5 Unbearable odor**

Intermediate ratings like 2.5 or 3.5 are also allowed.

The ratings are added up, the average calculated and mathematically rounded off to give a final rating. According to GUT, carpets with ratings below 4 have an acceptable odor.

This procedure has two main drawbacks. First, the analysis procedure is very expensive and time consuming. Secondly, the evaluation is by its very nature subjective. An annoying odor also represents an emotional impact, which varies depending on the situation and the emotional state of the person exposed

GERSTEL Headspace ChemSensor



to the odor; it is difficult to translate and generalize the results of a panel.

### Conventional electronic noses

The functional principle of a conventional electronic nose (E-Nose) is modelled on human olfactory sensory perception and processing.

E-Noses have an array of electrochemical sensors with some selectivity. These sensors assume the task of olfactory cells, their combined responses are recorded as a signature or fingerprint of the vapor sample in question. Data are transmitted to the „brain“ or processor of the sensor; the numerical sample recognition parameters are converted to an understandable signal by chemometric analysis; E-noses can recognize simple

Table 1: Tolerance levels of emission released from carpets with a GUT-signet

Component	Residual amount ( $\mu\text{g m}^{-3} \text{h}^{-1}$ )
4-VCH	2
Styrene	5
4-PCH	20
Toluene	50
Sum of aromatic hydrocarbons	150
TVOC (total volatile organic compounds)	300

and complex odors. There are presently three types of sensor that are used in conventional E-noses<sup>6</sup>:

- 1. Metallic Oxide Gas Sensors (MOS)**
- 2. Field Effect Gas Sensors (MOSFET and MISFET)**
- 3. Conducting Polymer Gas Sensors**

Traditional gas sensors have a number of disadvantages among which are a sensitivity to changes in relative humidity and temperature. Signal drift also occurs due to poisoning or due to oxidation in more polar sensor materials or coatings. Due to these factors, frequent and extensive calibration is required. Based on experience with conventional E-nose equipment, a choice was eventually made to not use such technology for this study.

### Headspace ChemSensor

The problems generally associated with conventional E-Noses can be avoided by using the technology forming the basis of the GERSTEL Headspace ChemSensor System. In the GERSTEL ChemSensor, which was introduced in 1998, a mass-spectrum fingerprint of a sample is obtained using quadrupole mass spectrometry. A headspace autosampler is used to condition the sample, collect vapors from the area around the sample and introduce the headspace vapors into the ChemSensor System. The headspace ChemSensor is thus based on headspace mass spectrometry with no gas chromatography (GC) separation; spectra of the odor as part of the total emission are collected and recorded.

### ChemSensors must be trained prior to use

Just like the human nose, the ChemSensor has to be trained to recognize odors. This is achieved by first analyzing a large series of known samples ranging from good to bad. Using the recorded data, models are created for the prediction of the odor of unknown samples. The chemometrics software can process a large amount of statistical data. The comparison of a large number of sensory fingerprints requires a high-quality sample recognition technique based on chemometric calculation models. Some of the models used are:

- 1. Principal Component Analysis (PCA)**
- 2. Hierarchic Cluster Analysis (HCA)**
- 3. Soft Independent Modelling of Class Analogy (SIMCA)**
- 4. Neural Network Analysis (NNA)**
- 5. K Nearest Neighbours (KNN)**

### Experimental

A GERSTEL ChemSensor system was used for the analysis of odors from carpets (see page 16, Fig. 4). The system uses a quadrupole mass spectrometer operated in Electron Ionization (EI) mode. Fingerprint-like total mass spectra are obtained, which provide the chemical background for the analysis of odors. The results obtained using ChemSensor were compared with the results obtained from the sensory panel.



Figure 2: Olfactory analysis by a sensory panel

**Table 2:** Olfactory analysis by a sensory panel

Parameters	NST 3320	ChemSensor
Sample preparation	Emission-free room	
Sample quantity	6 specimens of 10 mm diameter	
No. of analyses per sample	3	3
Incubation temperature	37 °C	90 °C
Incubation time	60 min	45 min
Sampling volume	60 mL / min	standard (2 ml loop)
Sampling time	45 s	standard (20 s)
Carrier gas	-	helium
Reference air	humidified synthetic air	-
Collection of baseline signal	30 s	-
Recovery of sensors	360 s	-
Flush time of needle	100 s	-
Mass range	-	50 to 200 amu

## Results

From January 2000 to December 2001, 1,000 carpet samples were analyzed using chemical sensor systems and an olfactory panel in parallel. The data collected were used to optimize the E-nose and the ChemSensor and to train them to predict odor perception of unknown carpet samples.

## Olfactory panel

The olfactory panel analyzed a total of 1,283 carpet samples (Fig. 5). The result was that 18 % were denied the GUT mark, 27 % met the requirement with an olfactory rating of 3.5, and 55 % of the samples were given the rating 3, reflecting an acceptable odor. As almost all carpet samples emitted a more or less pronounced „new carpet“ odor, the ratings 1 or 1.5 were rarely obtained.

## Chemical Sensor

The GERSTEL Headspace ChemSensor was trained with 200 samples and validated with 100 samples. As the ratings 1, 1.5, 2, 4.5 and 5 were missing, training was continued with the GUT limiting values as criteria (Fig. 5). Samples with a rating of 4 or worse were

rejected, samples with better ratings were accepted. In this case a classification model is needed with two classes: acceptable (ratings 1-3) and rejected (ratings 4-5).

## Creation of models

The first models were created with SIMCA. This chemometric method is based on PCA and so uses principal components and not actual variables. The accuracy of predictions was 80 %.

Better results were obtained with KNN. This method seeks the K-next neighbour in the space that is formed by all variables; in this case the 151 dimensional space with all fragments of the mass spectrum.

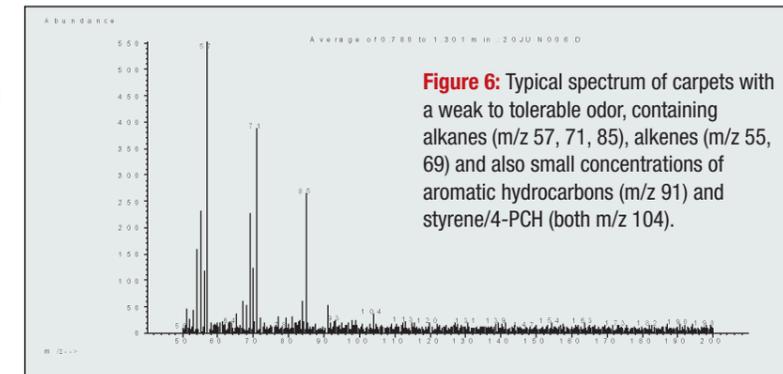
Using a KNN model with K = 4 and standardized data, 95 % of the samples were correctly classified, 5% were classified as bad. The majority of the samples were more exactly classified by the ChemSensor than by the olfactory panel; the accuracy of predictions was an actual 99 %.

## The source of the odor problem

Because the ChemSensor uses the total emission spectrum of the sample as a fingerprint, it reveals important information about the source of the odor. The total emission spectrum is a combined mass spectrum of all components being emitted, which cannot be used for quantitative analysis.

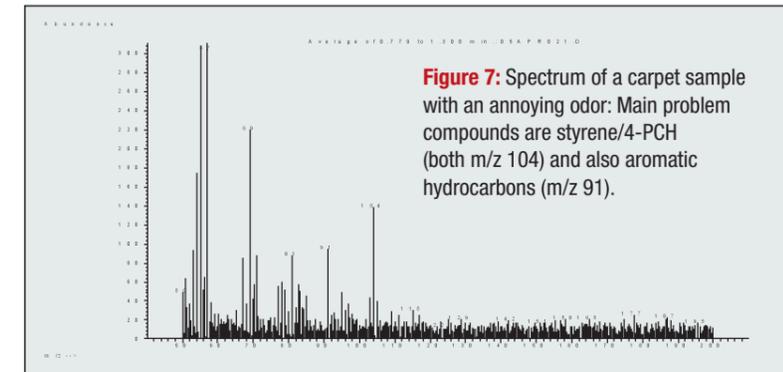
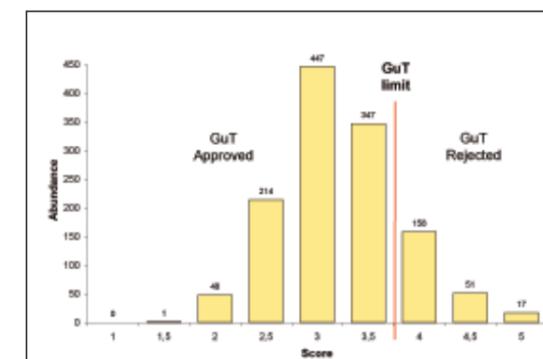
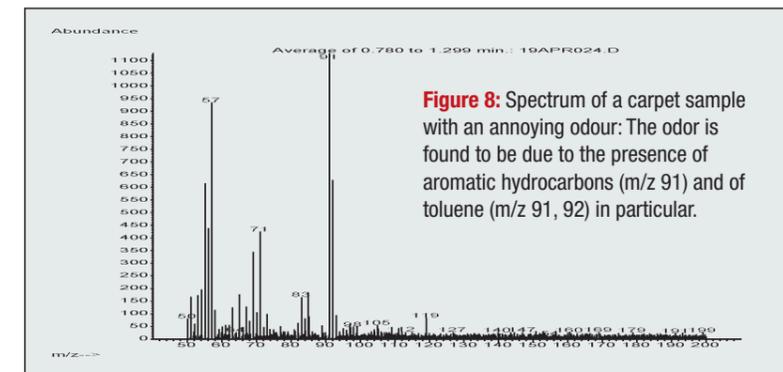
Qualitative analysis of unknown samples was initially found to be difficult, and in general limited to a comparison of samples. Over the past decade, however, knowledge about emission and about odor-causing compounds in carpets has increased.

Using this information, the total emission spectrum can be interpreted and used to obtain an indication of the source of the odor problem.

**Figure 4:** GERSTEL ChemSensor System**Figure 6:** Typical spectrum of carpets with a weak to tolerable odor, containing alkanes (m/z 57, 71, 85), alkenes (m/z 55, 69) and also small concentrations of aromatic hydrocarbons (m/z 91) and styrene/4-PCH (both m/z 104).

The ChemSensor proved valuable in evaluating and identifying sources of odor in samples which were misclassified or those which were borderline concerning GUT approval. If a rating of 3.5 or 4 was given, a further evaluation was possible using the ChemSensor.

Figure 6 shows the typical spectrum of a carpet sample with a weak odor (rating 2.5). The spectra in Figure 7 and 8 are from samples with an annoying odor caused by the presence of aromatic hydrocarbons (m/z 91) and a combination of styrene and 4-phenyl-cyclohexene (4-PCH). Both these compounds have a major fragment at m/z 104.

**Figure 7:** Spectrum of a carpet sample with an annoying odor: Main problem compounds are styrene/4-PCH (both m/z 104) and also aromatic hydrocarbons (m/z 91).**Figure 5:** Analyses by the olfactory panel in the years 2000 and 2001**Figure 8:** Spectrum of a carpet sample with an annoying odour: The odor is found to be due to the presence of aromatic hydrocarbons (m/z 91) and of toluene (m/z 91, 92) in particular.

## Long term odor emissions

To examine how long emissions and odors endure, eight carpets were cut to a defined size and the pieces stored for seven months under different conditions:

- 1) Unprotected at room temperature.
- 2) In mechanically closed polyethylene bags at a room temperature b) 5 °C and c) -20 °C. During the first month, samples were analyzed twice weekly, in the second month once weekly and in the third and fourth months every 14 days, thereafter once per month.

Data analysis with PCA showed a change over time for all storage methods, leading to change in fingerprint; the greatest change was shown in the samples left unprotected at room temperature, a similar change was seen in the samples stored in polyethylene bags at room temperature. The samples stored at 5 °C and -20 °C showed better results and were subsequently examined by the olfactory panel.

## Acknowledgement

This work was supported by the Belgian Government, the three Belgian Regional Governments, GUT and the Belgian Carpet Industry.

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**Pesticide analysis**

# A novel, fast technique with ultra-low detection limits

Pesticides protect vital crops and ensure abundant healthy food supplies. Anyone criticizing the use of pesticides in agriculture should remember that. Pesticides are an efficient way to control harmful insects and micro-organisms in agriculture. The use of pesticides has helped ensure better yield for farmers as well as higher quality and lower prices for consumers. However, pesticides pollute our air, soil and water. They contribute to the global loss of biodiversity and can have an adverse effect on human health. Every year, more than 30,000 tons of many different pesticides are spread on fields in Germany and 600,000 in the U.S.A. 250 active compounds and 1,900 products are approved in Germany, but far more are actually available.

**GERSTEL Twister Desorption Unit (TDU)**

Chemical compounds are extracted by the Twister and then desorbed by the Twister Desorption Unit (TDU).



»Fast and reliable, applied without any major sample preparation work and no solvents.« Ralf Bremer, GERSTEL's Technical Director explains the new screening system.

Improper application as well as the illegal use of banned pesticides are the biggest causes of concern. Since supply and distribution is difficult to control, the only way to provide effective protection of the environment and of consumers is to constantly monitor pesticide concentrations.

**The challenge of efficiently monitoring pesticide levels**

Environmental samples as well as food products need to be checked for pesticide traces on an ongoing basis. To help perform this service, there has been a constant search for improved methods of analysis, which can quickly determine if a sample is contaminated or not. In view of the fact that there are roughly 600 pesticides in circulation around the world, the analytical challenge is exceptionally difficult, due in particular to their different chemical and physical properties.

The standard analytical methods that are currently in use are laborious, time-consuming and costly. In addition, these methods require large amounts of solvents, some of which are toxic. In order to enable quick and sensitive determination of pesticides in a sample, GERSTEL has joined with the Research Institute for Chromatography (RIC) in Belgium to develop a new screening method, which was presented at Pittcon 2003 in Orlando, Florida, USA.

**An innovative and revolutionary solution**

The method is based on Stir Bar Sorptive Extraction (SBSE), a sample preparation method developed at the RIC, that is comparable to Solid Phase Micro Extraction (SPME) (see also page 2/3). The difference is that analyte extraction in SBSE is carried out with the GERSTEL Twister, a patented magnetic stir bar coated with a layer of polydimethylsiloxane (PDMS) 0.5 to 1 millimeter thick. „The phase ratio, i.e. the volume of the water phase to the volume of the PDMS phase, is considerably lower than in SPME, improving detection limits by up to a factor of 1000“, says Ralf Bremer, Technical Director of GERSTEL.

The components absorbed in the Twister can be desorbed thermally in a similar way to SPME for transfer to a gas chromatograph. The instrument system used for the analysis is comprised of the GERSTEL Twister Desorption Unit (TDU), the GERSTEL Cooled Injection System (CIS 4), and a GC/MS system with Retention Time Locking (RTL) software from Agilent Technologies.

„What this provides is a database that contains all the necessary information to determine 567 pesticide active compound by GC/MS, 440 of which we have already covered with our system“, explains Ralf Bremer. „Our

method is fast and reliable, it can be applied without any major sample preparation work and it requires almost no solvent.“

Using the GERSTEL MultiPurpose Sampler (MPS), up to 196 Twisters can be desorbed automatically, allowing pesticide contamination levels to be determined reliably, efficiently and within a very short time. „We are hopeful that this new technique will allow contaminated food products to be taken out of circulation before they are consumed, while laboratory personnel and the environment avoid unnecessary contact with solvents“, the director points out.

**GERSTEL Thermal Desorption System TDS**

## Proven Thermal Desorption System now offers analysis of passive sampling tubes

The latest TDS 2-7 model handles a number of different tube types, increasing the overall flexibility and productivity of the system. Passive sampling tubes from different manufacturers, including the widely used 1/4"x 3.5" tubes, can now be processed automatically using the TDS A2 Autosampler coupled with the TDS 2-7. The TDS system is the only system capable of analyzing such a wide variety of sampling tubes. The user benefits: Established methods using available tubes can be transferred to the proven, high-performance TDS 2-7 system.

**The application range of the GERSTEL Thermal Desorption System (TDS)**

Existing TDS 2 users can upgrade their system to desorb passive sampling tubes, for which complete data bases of collection rates exist. The proven GERSTEL TDS continues to offer outstanding performance for thermal desorption analysis in a wide range of application areas, where customers have come to rely on its capacity for preconcentration and ultra-low detection limits.

Examples of application areas where the TDS can be used are: Environmental, Flavours and Fragrances, Pharmaceutical, Semiconductors, Automotive materials, building materials, as well as polymers and packaging. Desorption of adsorbent-based tubes or of Twister stir bars as well as direct thermal extraction of solids without sample preparation is performed in a fully automated system.

# Introducing children to chemistry at an early age

**Promoting talent in the new generation**

How can there be something in a glass that appears to be empty? Why does ice float on water? Why does a candle go out when you blow hard at it? Kindergarden children have an unrelenting desire to get to the bottom of everything. Question after question comes from their small mouths in endless succession, and many of the questions are guaranteed to be difficult for adults to answer!

It is evident that the questions they pose relate mostly to everyday things, and that they have a background based on physics or chemistry. „No wonder!“ says Gisela Lück, because after numerous informative trips to kindergardens countrywide, she came to the conclusion that „particularly five to six year olds really have the ability to grasp and remember natural science connections, and enjoy doing so“. Prof. Lück has been busy for over a decade studying whether, how and at which age it makes sense to explain



physical and chemical causes of everyday occurrences to children. Children ought to receive these explanations in a manner that stirs their interest in natural science as early as possible. To collect and evaluate sufficient relevant information, Prof. Lück actively worked in kindergardens for several years.

During this time 25 experiments were developed that „make natural science accessible and understandable – using all senses“. The experiments all meet the following requirements: „suitable for children, safe, inexpensive, possible to perform with simple household means and, above all, understood by children“. Using these experiments, a successful start to chemistry and physics can be made at the pre-school age. „Even children that are challenged mentally in speech or motor functions profit from the experiments“, says Gisela Lück.

„Prof. Lück's results have gained our attention and motivated us to promote scientific upbringing where it appears to be most effective, in the kindergarden“, explained Holger and Eberhard G. Gerstel, Managing Directors and Joint Owners of GERSTEL GmbH & Co. KG. The results of an exchange of ideas between Prof. Lück and the company were an open Info-Evening and a plan by the company to help teachers with continuing education. This was



**How the interest of children in natural science** can be aroused was the subject of a discussion between the owners of the company, scientists, politicians and educationalists from Muelheim on Ruhr at the GERSTEL company.

expressed by Holger Gerstel: „We will practice performing some of the experiments developed by Prof. Lück with groups of 15 teachers or less. Given appropriate instructions, teachers can include these experiments in their kindergarden games.“ „As part of society, we must assume responsibility“, Eberhard G. Gerstel added: „If we want a qualified new generation, we need to start promoting it at an early stage.“