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GERSTEL

ISCC 2010 Riva del Garda

Newsletter

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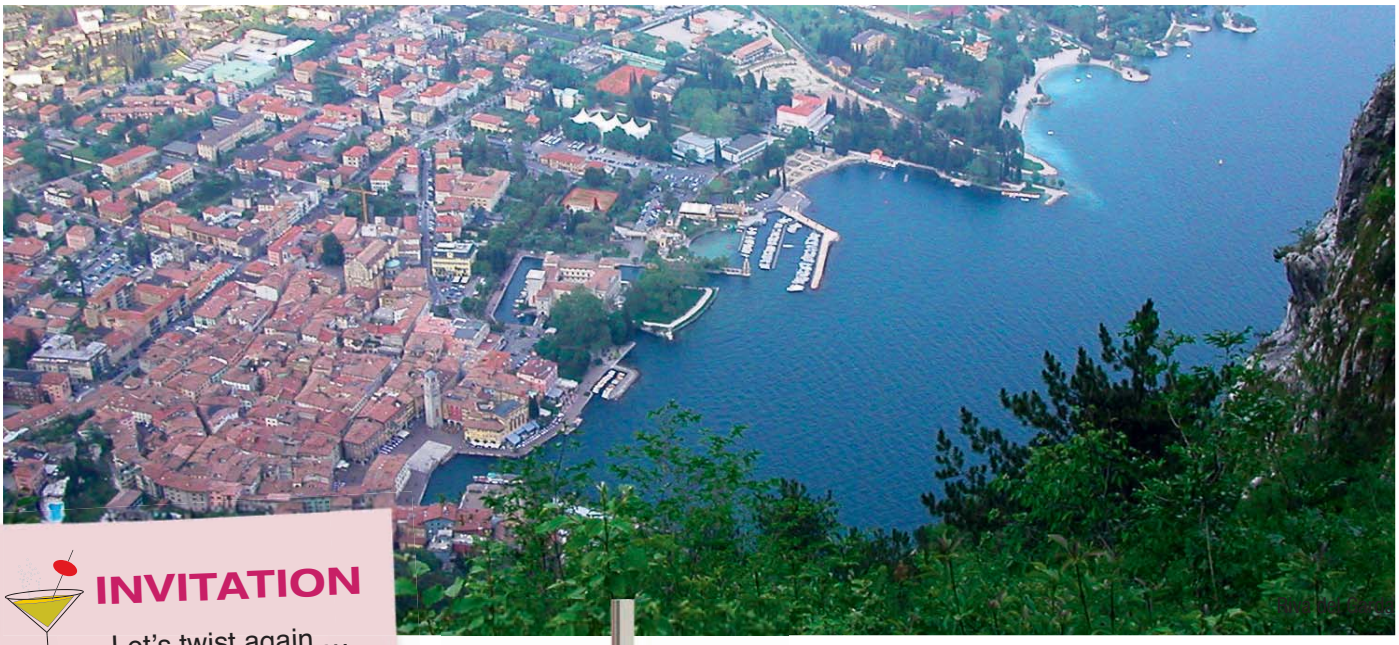
June 2010



INVITATION

Let's twist again …

Twister Cocktail Night
Tuesday, June 1, 2010
Starting 10.15 p.m.
Congress Center

Selectable 1D/2D GC/MS at ISCC 2010

An extra GC dimension at your finger tips

Gas chromatography (GC) experts rely on sharp peaks and baseline resolution to provide accurate answers. To perform chromatographic analysis of real-world samples, analysts often must deal with either complex sample types such as essential oils and petroleum fractions, or complex matrices like biological fluids, foods, sludge, or polymers. Once the sample has been prepared for analysis, separation of all the individual compounds present by means of a single chromatographic separation can be challenging due to the compounds having different ranges of polarity, boiling point, solubility, MW, and concentration. It is therefore necessary to use innovative yet robust techniques that go beyond using a single chromatographic dimension to achieve compound separation. This sounds simple enough, but until now it hasn't been, since techniques that require a second dimension (column) require a lot of additional hardware.

Not anymore: The patented GERSTEL Selectable 1D/2D-GC/MS System enables the best of both worlds. The system can be used for routine single dimensional GC/MS analysis, and with the click of a mouse, can be switched to perform two-dimensional separation when needed for more complex matrices. This allows interesting sections of the chromatogram to be collected and concentrated from multiple runs to better separate and isolate trace compounds. This can, for example, be used for trouble shooting when off-odors are detected in a product. All this is performed using just one GC/MS system.

Continued on page 2

GERSTEL Vendor Seminar

Wednesday, June 2, 2010,
15.45 – 16.45, Gerstel – Room 1000

New Applications of Automated Dynamic Headspace coupled to One-Dimensional and Two-Dimensional GC-MS
Christophe Devos, RIC, Belgium

Polar Phases for Stir Bar Sorptive Extraction - Possibilities and Limits
Eike Kleine-Benne, GERSTEL, Germany

Automated Pyrolysis GC combining a Filament Type Pyrolyzer with an Automated Thermal Desorption Unit
Carlos Gil, GERSTEL, Germany

Doing Drugs?

Automated DPX and LC/MS/MS with dynamic MRM. To learn more get the latest Solutions Magazine at the GERSTEL booth .....

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An extra GC dimension at your finger tips

Authors
Nobuo Ochiai, Ph. D., Technical Director,
Kikuo Sasamoto, Technical Manager,
GERSTEL K.K., Tokyo, Japan

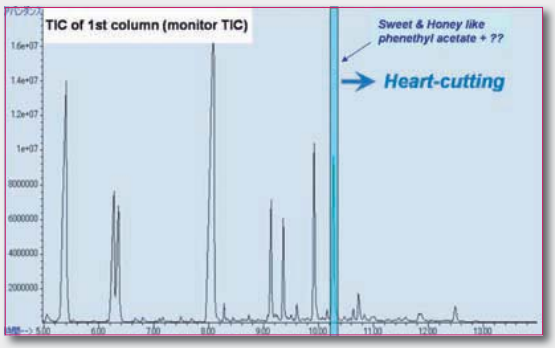
Food analysis is certainly not a trivial matter. The typical matrix is complex, often requiring several sample preparation steps and extensive sample clean-up. However, even well prepared samples can produce forests of overlapping peaks making it a case of not being able to see the trees for the forest. If a case of unresolved peaks is clearly at hand, or if an odor detected by using an Olfactory Detection Port (ODP) doesn't match the chromatogram, the user needs to have a good tool kit at her or his disposal. In this case, selectable multidimensional GC can be the technique that cuts through the thicket and provides clear, reliable answers whenever one-dimensional GC does not.

Until now, multi-dimensional GC required the use of a dedicated system with two GCs coupled to each other. Due to the extra cost, and to the often limited utilization in the laboratory, such solutions didn't always provide the best return on investment (ROI). GERSTEL now offers a solution that can be used for routine analysis as well as for special challenges. The patented GERSTEL Selectable 1D/2D-GC/MS is a flexible system, based on a single standard GC/MS instrument. It is both a routine analysis system and a complex problem solving system that offers heart-cutting and two-dimensional separation on demand. Because of this dual functionality, when questions arise regarding a section of the standard one-dimensional chromatogram, this section in question can be transferred to a 2nd dimension, i.e. a GC column with different polarity to further increase separation. Both columns are installed in the same GC and are heated independently using Low Thermal Mass (LTM) technology. The process of cutting a section of a chromatogram and introducing it to another col-

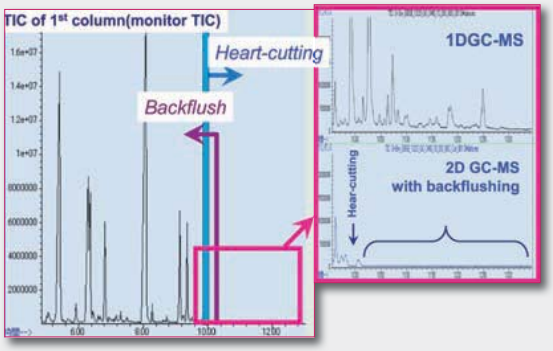
»The main advantages of the selectable 1D/2D-GC-MS system are the simple and fast selection of 1D GC-MS and 2D GC-MS operation with a mouse click (without any instrumental set-up change), and simultaneous mass spectrometric and olfactometry or element-specific detection for both 1D and 2D separation to assure selection of a heart-cut region and correct identification of compounds of interest.«

Nobuo Ochiai, Ph. D.
Technical Director, GERSTEL K.K.

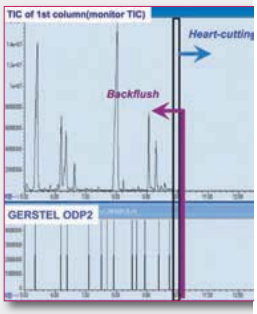
SBSE – 2D GC-O/MS determination of odor-active compounds in beer



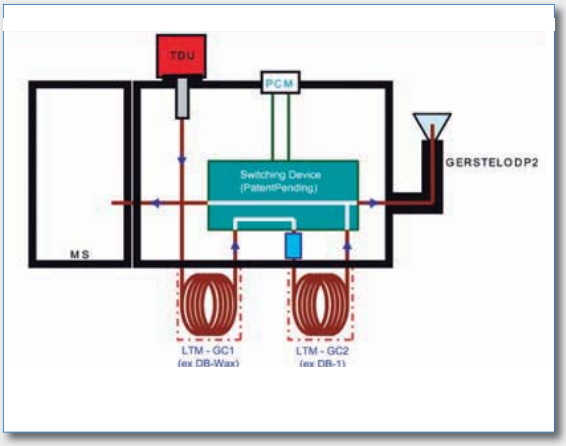
1D GC-O/MS analysis
GC-O/MS can help locate the region of odor-active compounds within a complex Chromatogram, but insufficient resolution may still prevent reliable compound identification. A heart-cut of the region of interest followed by separation on a second column (second dimensional separation) provides the resolution needed to accurately identify individual compounds.



Heart-cutting and Backflushing
The system can be configured to perfom 2D GC-O/MS analysis without any hardware or column connection changes. After heart-cutting, the 1st dimensional column can be backflushed. An additional cryo-trap device is available if necessary.



Simultaneous MS and olfactory detection is possible in both 1D and 2D GC analysis modes.



Selectable 1D/2D GC-Olfactrometry (O)/MS System

Heart-cutting
User selected peaks eluted from LTM-GC Column 1 are transferred onto LTM-GC Column 2. The transferred peaks are focused at the head of the LTM-GC Column 2 with or without cryo-trapping depending on the compound volatility.

»Also, this system can eliminate preliminary analysis with a "monitor FID" for the selection of the heart-cut region, and can provide a "monitor total ion chromatogram (TIC)" for the 1D column separation in 2D GC-MS analysis.«

Kikuo Sasamoto
Technical Manager, GERSTEL K.K.

umn is called heart-cutting. The 1D/2D system can be used to determine analytes in either the 1st or the 2nd dimension in a flexible manner. Neither the GC run, nor analyte detection is interrupted during the run. Detection of the analytes that were transferred to the 2nd column follows using the same detector(s) used for the 1st dimension: MSD, Olfactory Detection Port (ODP), PFPD etc. etc. Should lower detection limits be required for the analyte in question, the system enables heart-cutting from multiple repeat injection, with cryofocusing of the sections that were cut, on a GERSTEL Cryo Trap System (CTS). The accumulated sections are then transferred to the 2nd dimension once there is sufficient mass on column to perform the determination.

The complete system is efficiently and conveniently controlled by mouse-click through the GERSTEL MAESTRO software, integrated with the Agilent ChemStation. It couldn't be simpler.

For more information

www.gerstel.com,
e-mail: gerstel@gerstel.com

Literature

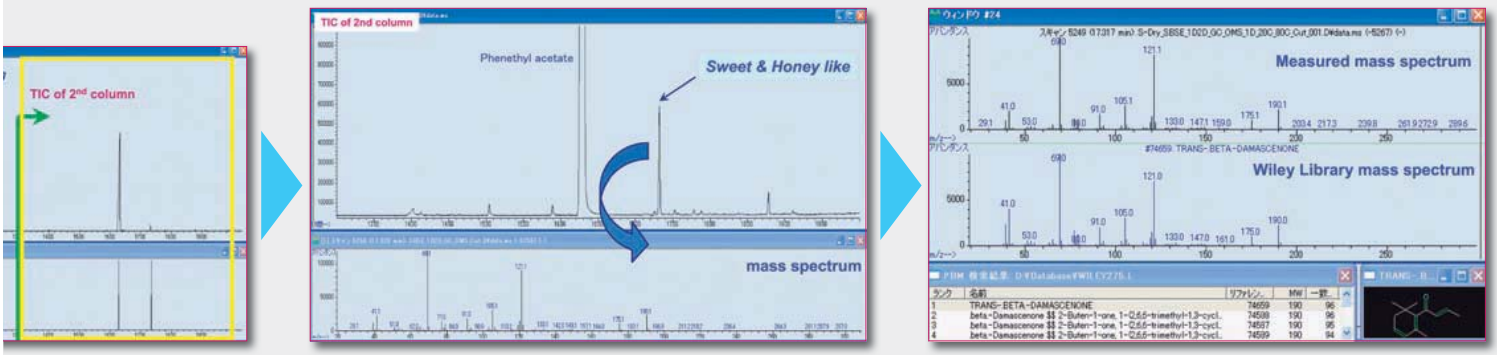
Kikuo Sasamoto, Nobuo Ochiai: "Selectable one-dimensional or two-dimensional gas chromatography-mass spectrometry with simultaneous olfactometry or element-specific detection", Journal of Chromatography A, 1217 (2010) 2903–2910.

A new sorbent phase enables selective extraction of polar compounds using the GERSTEL Twister®

New Twister for polar compounds

Stir Bar Sorptive Extraction (SBSE) using the patented GERSTEL Twister is an accepted and highly efficient extraction technique for the determination of organic compounds in aqueous and other samples. The recent introduction of a polyacrylate (PA) sorbent phase complements the standard phase, enabling more selective extraction of polar compounds. SBSE with the PA Twister is performed just like any other SBSE extraction: Place the PA Twister in the sample and allow it to stir for 20 minutes to one hour. While stirring, the Twister extracts polar compounds and concentrates these in the PA sorbent phase. The Twister is removed, rinsed with DI water, dried using lint-free paper tissue, and placed in a thermal desorption tube for desorption in a GERSTEL Thermal Desorption System (TDS) or Thermal Desorption Unit (TDU). Analyte focusing, separation and determination follows in the GC/MS system. The difference between the standard Twister and the PA Twister is not only seen in the chromatogram and in the analytical results, it is clearly visible to the naked eye. The PA sorption phase is placed on a solid support, which is placed around the Twister's glass encased magnetic core. The combination of solid support and polyacrylate sorbent has proven to be easy to produce and stable during thermal desorption. The PA Twister is especially convincing when performing selective extraction of phenols and other compounds that form hydrogen bonds.

Financial support by the German Ministry for Economics under the ProINNO II Grant KF 0189604VT is gratefully acknowledged.



2D GC-O/MS analysis
The peak of interest was well separated, and detected using olfactometry (ODP) on the second dimension. A well defined mass spectrum was obtained for the detected peak.

Library search
A Wiley library search tentatively identified the peak as a β-Damascenone.

New automated pyrolysis module based on the proven GERSTEL Thermal Desorption Unit (TDU) extends the analyst's toolkit for elucidation of macro-molecular structures using automated GC/MS

Automated Pyrolysis for GC/MS

Determining the structure of complex molecules and polymers is a task that puts high demands on analytical instrumentation and analyst alike. Pyrolysis is more often than not the method of choice or at least a key part of the process. The molecular structure is broken down in a controlled manner by heating the sample in the absence of oxygen. The resulting fragments are separated and determined using mass selective detection (MSD) or flame ionization detection (FID). By comparing the resulting chromatograms and MS spectra with library data, the molecular structure and the type of a sample material can be deduced. Equally, temperature programmed pyrolysis can be used to simulate thermogravimetric analysis and determine which compounds are released from the sample in the process.

At the ISCC 2010 in Riva del Garda, GERSTEL is introducing a novel pyrolysis module based on the GERSTEL Thermal Desorption Unit (TDU). The pyrolysis module can be integrated into

existing GC/MS hardware and software. The idea behind the project is to enable automation of the established GERSTEL pyrolysis technology based on the company's MultiPurpose Sampler (MPS), adding pyrolysis to a long list of automated sample preparation and introduction techniques for GC/MS.

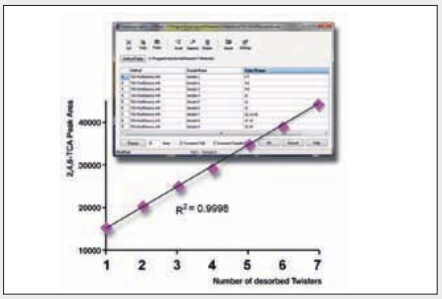
The automated pyrolysis solution based on the TDU enables the combination of all thermal desorption techniques and pyrolysis in one automated system. Temperature programmed or flash pyrolysis can be selected in the MAESTRO software. The pyrolysis temperature can be specified at values between 350 and 1000 °C. Up to 98 samples can be analyzed unattended in one batch.

The TDU in combination with the GERSTEL Cooled Injection System (CIS) is a highly versatile sample introduction system for GC/MS that covers almost every sample introduction technique. When needed, analytes released in the pyrolysis process can be concentrated for improved separation, sensitivity and limits of determination.

The GERSTEL TDU with pyrolysis option is a powerful addition to any GC/MS analysis system in the fields of research and development, quality control as well as forensic and polymer analysis. The system is operated from the MAESTRO software, stand-alone or fully integrated with the ChemStation from Agilent Technologies. Just one method and one sequence table are needed to operate the complete system from sample introduction to GC/MS analysis.

Multi-Desorption Mode TD

Automated Multi-Desorption Mode is available for the GERSTEL Thermal Desorption System (TDS) and GERSTEL Thermal Desorption Unit (TDU). Analytes from several sample



extractions can be desorbed and concentrated into one GC/MS run, significantly increasing sensitivity and reducing limits of determination. Multi-desorption mode is activated by simple selection in the MAESTRO configuration editor. In the sequence table, desorption of multiple adsorbent tubes or Twisters for every GC/MS run can then be specified. Individual tube numbers or ranges can be chosen freely. For SBSE analysis, system sensitivity has been shown to be proportional to the number of Twisters desorbed. For more information about Multi-Desorption mode and other GERSTEL solutions, please contact GERSTEL: gerstel@gerstel.com or visit our website: www.gerstel.com

GERSTEL LC/MS Effluent Optimizer (LEO)

In LC/MS, we work hard to reach the goal of achieving the perfect LC separation and combining it with the most efficient ionization and lowest achievable MS detection limits for our analytes.

The LC separation may require a certain pH and polarity range of the eluent, while analyte ionization in the LC/MS ionization source requires yet another pH, a different buffer – or even derivatization of the analyte for best possible efficiency or optimized spectral information. How to optimize both? The logical answer is to take the effluent from the perfect LC separation and optimize it for MS analysis.

This task is easily possible when you add the GERSTEL LC/MS Effluent Optimizer (LEO) module to your LC/MS/MS system. Application examples show sensitivity gains of up to a factor of 40 by simply adding a salt solution to the LC effluent and/or changing its pH. The LEO module is quickly and easily installed in your LC/MS system. A solvent mixture, buffer solution or reagent is then easily added to the effluent ensuring that the LC separation can be performed under optimal conditions while also enabling maximum yield in the MS ionization process, helping to reduce or eliminate Ion Suppression. Whether you are looking to perform pH adjustment or post-column derivatization, for method development or routine analysis, when you use LEO and the GERSTEL MAESTRO software you can easily and efficiently control all parameters as part of the overall method. Just one sequence table controls the entire system from sample preparation through LC separation and effluent optimization to MS analysis. It is all done with the click of a mouse.