

# FlavourSpec<sup>®</sup>

Gaschromatograph-Ion Mobility Spectrometer



**GC-IMS for the Detection of Volatile Organic compounds in Food and Beverages**

## FlavourSpec® – Your fast and easy-to-use tool for Food Control

The FlavourSpec® represents the synergies of a fast gas chromatograph and the outstanding sensitivity of an IMS. It enables the selective detection of Volatile Organic Compounds (VOCs) in the headspace of solid and liquid samples. As result a 3 dimensional spectra as characteristic fingerprint of the sample is achieved and further analyzed using multivariate data analysing tools. To make the operation of sampling and processing simple and easy the system is set up with an automatic GC headspace injector.

### Features

- Automatic GC headspace injector
- Stand-alone system with integrated computer
- Heated IMS, column, lines (< 80°C)
- Purification mode
- Access to all relevant parameters for method development: Temperature control of IMS, column, injector, drift and carrier gas flow rate
- Software controlled switching between positive and negative ionization mode
- Manual or fully-automatic operation incl. data acquisition, -analysis and visualization
- Storage of data on internal memory or external network shares and transfer to external devices
- PC-Software package

### Applications

- Control of storage conditions
- Food freshness
- Control of production process
- Process optimisation
- Flavour evaluation and flavour stability
- Test of raw materials
- Product authentication

### Technical Specification

**Working principle:** Ion Mobility Spectrometry (IMS)

**Ionisation:**  $\beta$ -radiation source (Tritium ( $^3\text{H}$ ))

**Activity:** 300 MBq, below the exemption limit of 1 GBq, EURATOM guideline

**Drift voltage polarity:** Positive and negative, switchable

**Sampling:** Automatic GC headspace injector

**Detection limit:** Low ppb<sub>v</sub>

**Dynamic range:** 1-3 orders of magnitude

**Display:** 6.4" TFT, VGA-Display

**Input unit:** Rotary pulse encoder

**Processor:** 400 MHz X-scale

**Data acquisition:** Ultra-fast ADIO-board

**Data processing:** X-board / Baseboard

**Data storage:** 2 GB Compact-Flash

**Communication:** RS232, USB, Ethernet

**Electrical connectors:** 2 x D-Sub 9-pole (for modem, console), D-Sub 15-pole (for external devices), RJ45 (for digital modem or SSH), 2 x USB-A

**Power supply:** 100-240 V AC, 50-60 Hz (external supply), 24 V DC / 5A, XLR-connector (internal)

**Power consumption:** < 180 Watt

**Dimensions:** 449 x 375 x 177 mm (WxDxH)

**Weight:** 15.5 kg

**Housing:** 19" compatible, IP 20 enclosure, EMC certificated

**Gas connectors:** 3 mm stainless steel Swagelok connectors for gas in- and outlet

### Automatic headspace sample injector headspace

**Features:** Incubator oven, agitator and heated gastight syringe

**Sample capacity:** 32 or alternatively 96 vials (10 or 20 mL)

**Operation:** Control panel with 4 function keys, graphic display, scroll knob for steering

**Dimensions:** 828 x 385 x 648 mm (WxDxH)

**Weight:** 10 kg







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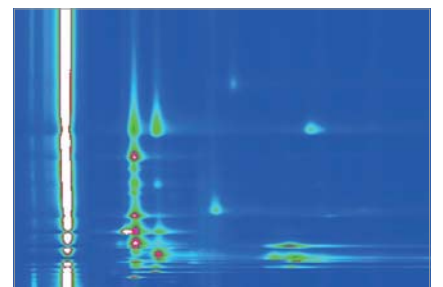
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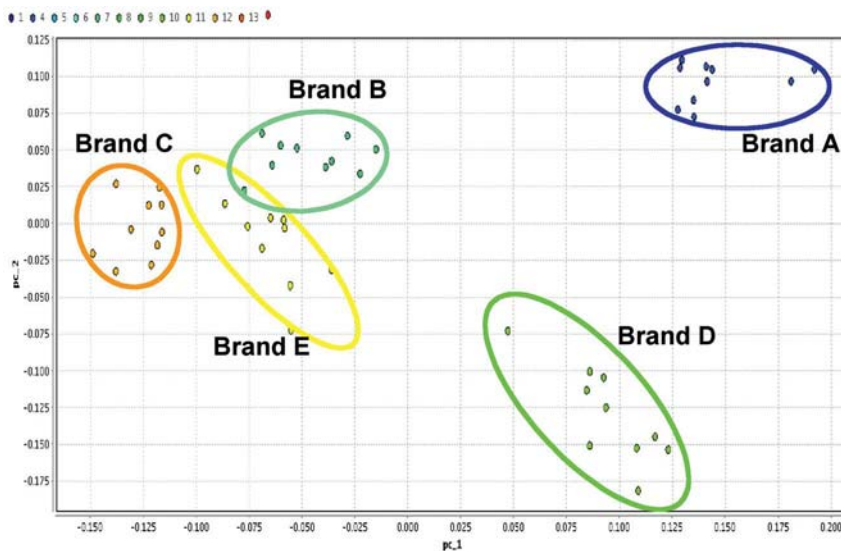
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## Freshness of Fish

The FlavourSpec® allows an easy and fast control of the storage conditions of food and beverages due to a “fingerprint” / pattern analysis taken from the sample’s headspace. Volatile induced flavours of fish samples were periodically (every 3 hours) analysed during storage at room temperature (20°C).

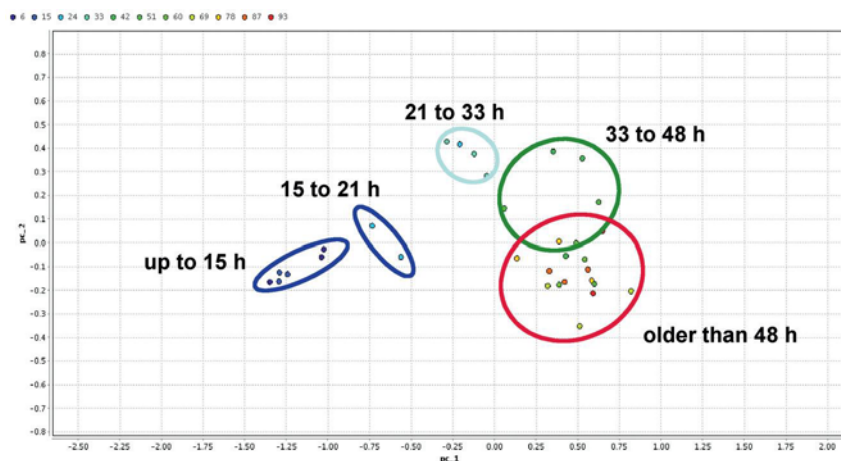
Quality degeneration of the sample could be detected and easily monitored by using the FlavourSpec®.



FlavourSpec®

FlavourSpec®
Total analysis run time: 3 minutes
Column type: MCC - 20 cm length, OV5
Column Temperature: 40 °C
Column carrier gas flow rate: 28 mL/min
Drift gas flow rate: 500 mL/min
Drift gas / Carrier gas: Nitrogen 5.0 (99.999%)
IMS temperature: 45 °C
Injector temperature: 80 °C

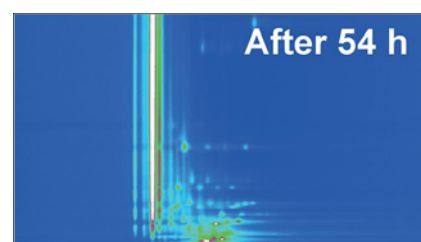
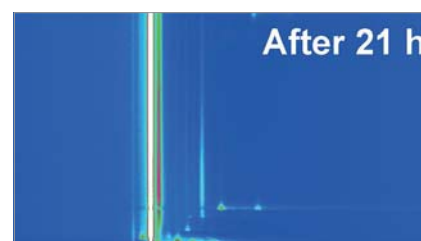
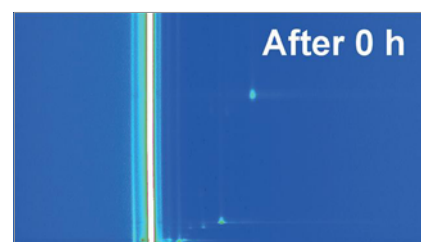
Automatic headspace sample injector
Sample capacity: 32 x 20 mL vials
Syringe cleaning: Inert gas purging of heated syringe
Incubation time: 5 min
Incubation temperature: 60 °C
Control: Easy-in-use handheld controller



Classification



Fish



Topographic plot of IMS Chromatogram

## Discrimination of Olive Oils

The FlavourSpec® allows an easy and fast quality control of food and beverages due to a “fingerprint” / pattern analysis of samples taken from the headspace.

Flavours of different types of olive oils were analysed and a good spectra differentiation hence authentication without any sample preparation or treatment could be achieved.



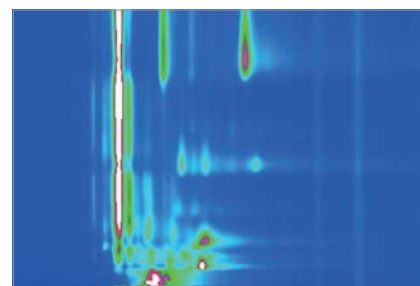
FlavourSpec®

<b>FlavourSpec®</b>
Total analysis run time: 3 minutes
Column type: MCC - 20 cm length, OV5
Column Temperature: 40 °C
Column carrier gas flow rate: 18 mL/min
Drift gas flow rate: 500 mL/min
Drift gas / Carrier gas: Nitrogen 5.0 (99.999%)
IMS temperature: 45 °C
Injector temperature: 80 °C

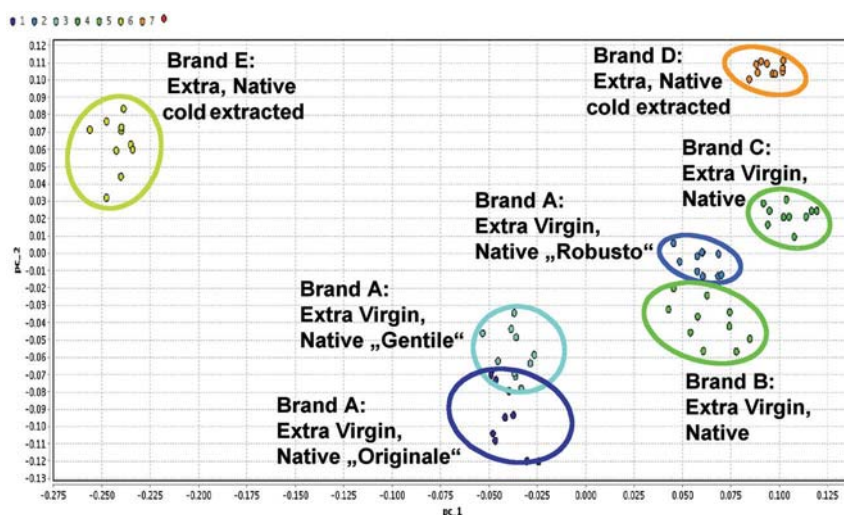
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Olive oil



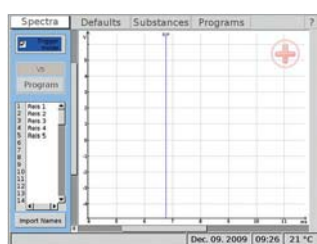
Topographic plot of IMS Chromatogram





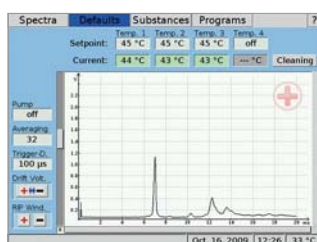
## Firmware of FlavourSpec®

The FlavourSpec® carries an in-system computer unit that allows to operate the device as a stand-alone unit. Its key advantage is its user friendliness due a self explaining menu. Operational steps as well as settings of a measurement are visualized on the 6.4" TFT display and can easily be executed or changed through a rotary pulse encoder.



### Spectra window

- Displays current spectrum
- Start/Stop command: Manually executed or by predefined programs
- Upload of sample name lists
- Set of external trigger e.g. to start autosampler



### Defaults window

- Set of temperatures (IMS, sample loop and inner tubes)
- Adjustment of pump, averaging and trigger duration
- Switching of drift voltage polarity
- Set of area for Reaction Ion Peak (RIP) determination



### Substance window

- List of substances with their
  - Relative drift time ranges
  - Elution time range (retention time)
  - Polarity
  - Alarm threshold



### Program window

- Definition of programs (actions at certain spectra number):
  - Valve switching
  - Data recording
  - Pump value
  - Temperatures



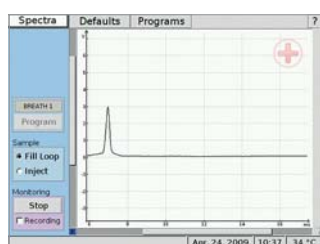
### Set up & Info "?" window

- Data download (Lan connection / USB)
- Device plan
- Display settings
- Internal parameters
- Firmware upgrade
- General information (Serial number, IP address, Software version etc.)



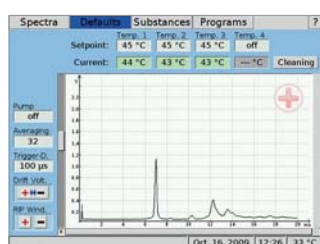
## Firmware of MCC-IMS / UV-IMS / A-IMS

All G.A.S. devices carry an in-system computer unit and can be operated as stand alone devices. They show outstanding user friendliness through a self explaining menu. Operational steps as well as settings of measurements are visualized on the 6.4" TFT display and can be executed or changed by a rotary pulse encoder.



### Spectra window

- Displays current spectrum
- Start/Stop of measurements: Manually executed or by predefined programs
- Manual injection



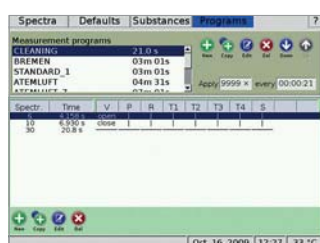
### Defaults window

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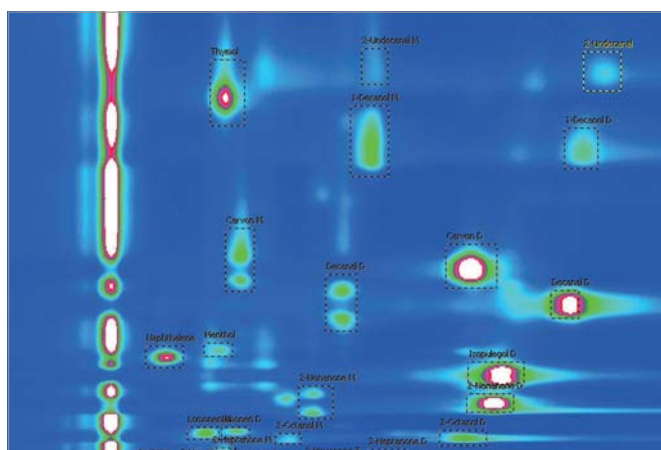


### Set up & Info "?" window

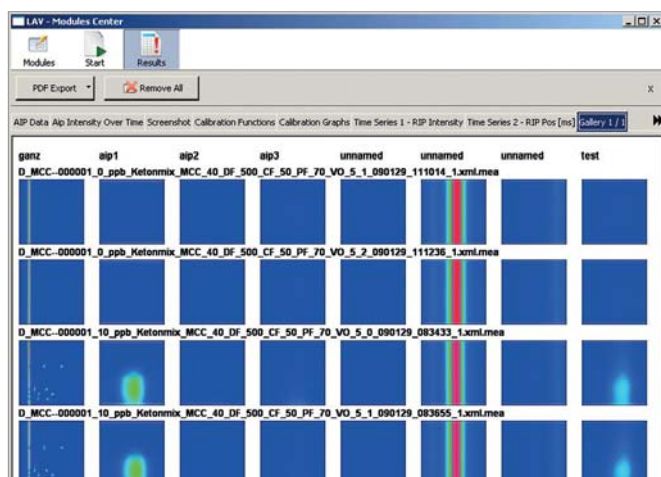
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## Data Processing of Ion Mobility Spectrometers (IMS) made by G.A.S. mbH

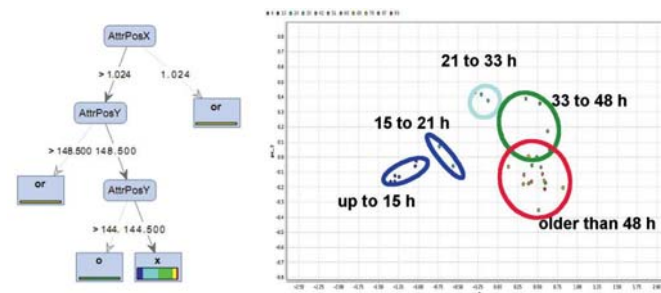
Fast and easy-in-use analytical tool – just a view steps to obtain a result using G.A.S.' instruments:



Topographic plot of IMS Chromatogram



Data extraction



Decision tree

Classification

### 1) Measurement Acquisition

During the training phase, the headspace of a sample with a known classification is introduced into the system and analysed. The resulting IMS chromatograms show the fingerprint of the compounds inside.



### 2) Learning

Main parameters of the complex data set are extracted either by the user or automatically. Based on these data a model/method can be developed for further classification of unknown samples.



### 3) Prediction / Classification

The prediction mode allows to use the IMS Chromatogram for further unknown samples and compare them with the developed models/methods. The results for classification/authentication are displayed.