



Mass Spectrometry Instruments

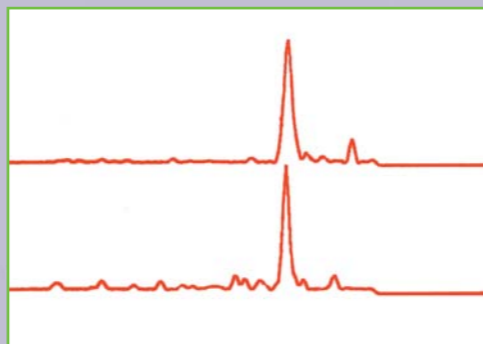
providing high performance instrumentation for the analytical world

AUTOCONCEPT

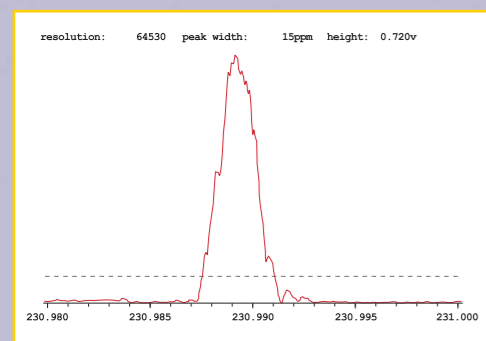
World class mass spectrometry providing high performance for the most exacting analyses

The Benefits of High Performance

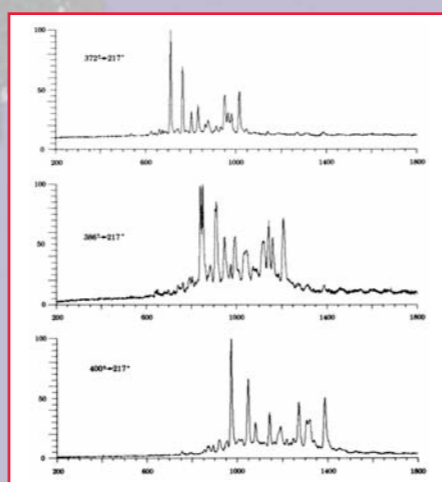
The high performance capability of Autoconcept provides the user with a distinct advantage - high sensitivity, resolution, selectivity and specificity. Take mass measurement for example. It is easy to measure a mass peak at low resolution - in theory the mean point of the ion distribution provides an accurate result. However, problems invariably occur when interfering ions at the same nominal mass distort that mean point. That's where the resolving power of Autoconcept can exclude those interferences resulting in an accurate mass you can have confidence in. Similarly, when monitoring environmental contaminants, the resolution of Autoconcept can tune out interferences and, by increasing selectivity and specificity, result in overall higher sensitivity with absolute confidence in the results.



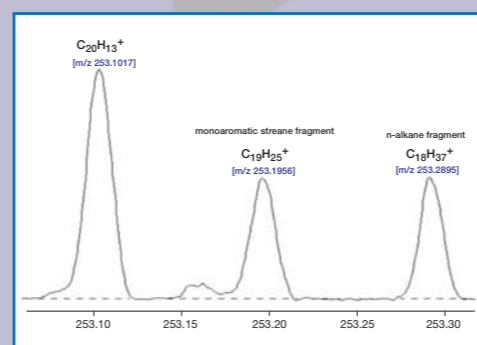
Sensitivity:
High sensitivity ensures a high signal-to-noise ratio in analyses such as this 50 fg detection of dioxin at m/z 320 and 322



Resolution:
Autoconcept is specified to greater than or equal to 80,000 resolution using the 10% valley definition, unlike other MS technologies which use a 50% definition.
Note: The resolution displayed here is equivalent to over 120,000 in 50% definition terms



Selectivity:
The ability to use high performance MS characteristics to select only ions of interest is shown clearly in this multiple chromatogram of sterane distributions in shale oil. Metastable ion monitoring techniques have been used to separate the 3 sterane species unambiguously



Specificity:
High performance provides superior identification capabilities. The spectrum above presents ions in an oil sample with the same nominal mass of 253. Autoconcept can successfully separate the individual ionic species



HIGH PERFORMANCE

Designed for high sensitivity, reproducibility and reliability in high resolution applications

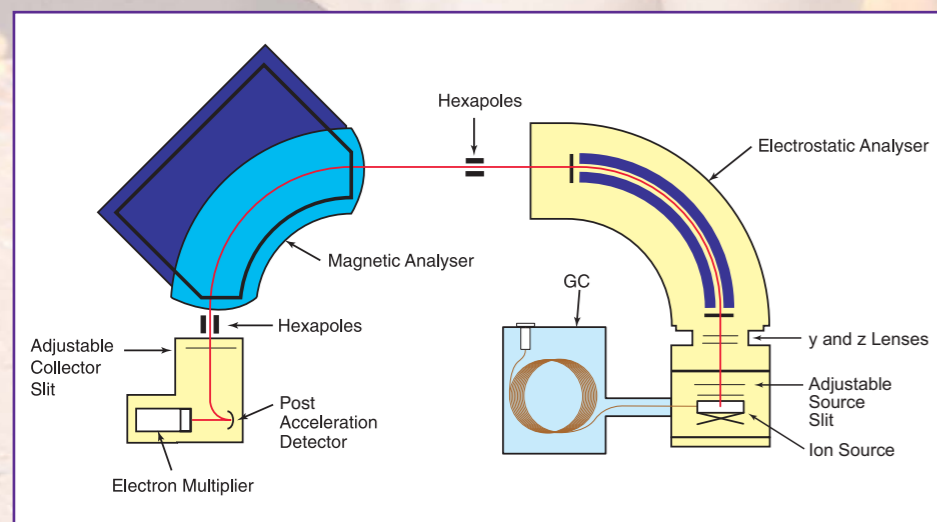
The Autoconcept is a high performance mass spectrometer dedicated to the analysis of organic materials to provide accurate mass information.

The instrument features a horizontal, E-B geometry mounted on a solid framework with a three point anti-vibration support system, resulting in a highly stable instrument capable of achieving ultimate detection levels in a reproducible and consistent manner.

When Less Gives More

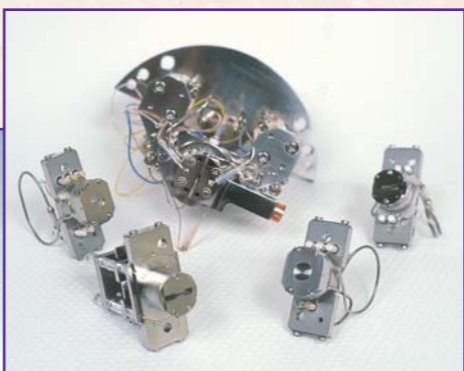
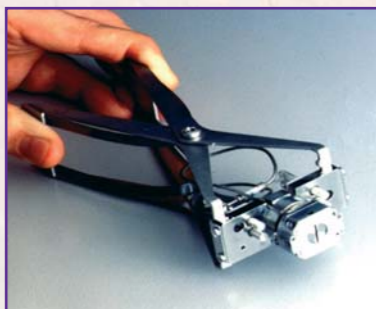
Autoconcept's ion optics involve high precision engineering yet the design has produced a very simple layout with very few focusing lenses. All mass spectrometers use focusing lenses to ensure that the ion beam remains in the correct orientation. As all lenses have an element of interaction with each other then it is clear that the fewer the lenses, the easier the operation of the instrument. As a result of its superior basic ion optic design, Autoconcept has many benefits:

- **Autotuning is fast and easy**
- **Calibration is very stable**
- **Resolution is maintained over long periods**
- **Ultimate performance is guaranteed**



Multi-purpose Flexibility

The sheer ease of source changes, the availability of multiple inlet systems and the reliability and stability of Autoconcept allows the instrument to be used in multi-purpose environments.



Ion Optics:

The simple high precision ion optics of the Autoconcept result in an instrument which has high stability, sensitivity and resolution

Sources:

Autoconcept features a wide range of source configurations - all with the innovative rapid clip-in connection system



With Dedicated Performance

Autoconcept S Series is ideally suited to dedicated analyses, particularly those with the exacting requirements of environmental monitoring such as the dioxin and furan methods specified by USEPA1613 and EN1948.

Autoconcept H Series features an inhomogeneous field magnetic sector. This provides for a mass range up to 10,000 daltons at full sensitivity. Combined with techniques such as LSIMS and field desorption, and with its high efficiency detector, Autoconcept H Series is ideal for high resolution analysis of high mass biological materials such as peptides, proteins and oligosaccharides.

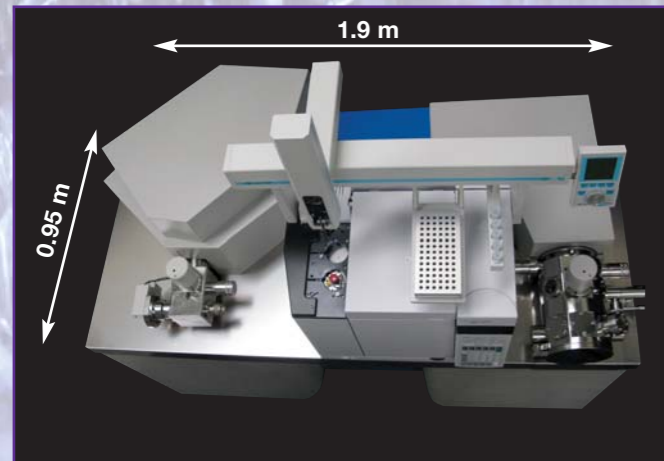


ENVIRONMENTAL

The latest Autoconcept provides highest performance with the ease-of-use and flexibility necessary for modern environmental laboratories

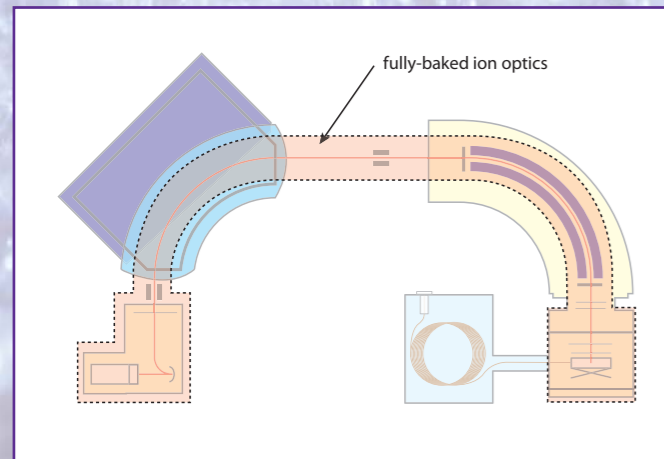
Compact Instrumentation

The Autoconcept features the smallest footprint of any instrument in its class.



Smallest Footprint:

With space a premium in analytical laboratories, Autoconcept requires less floorspace than other instruments in its class

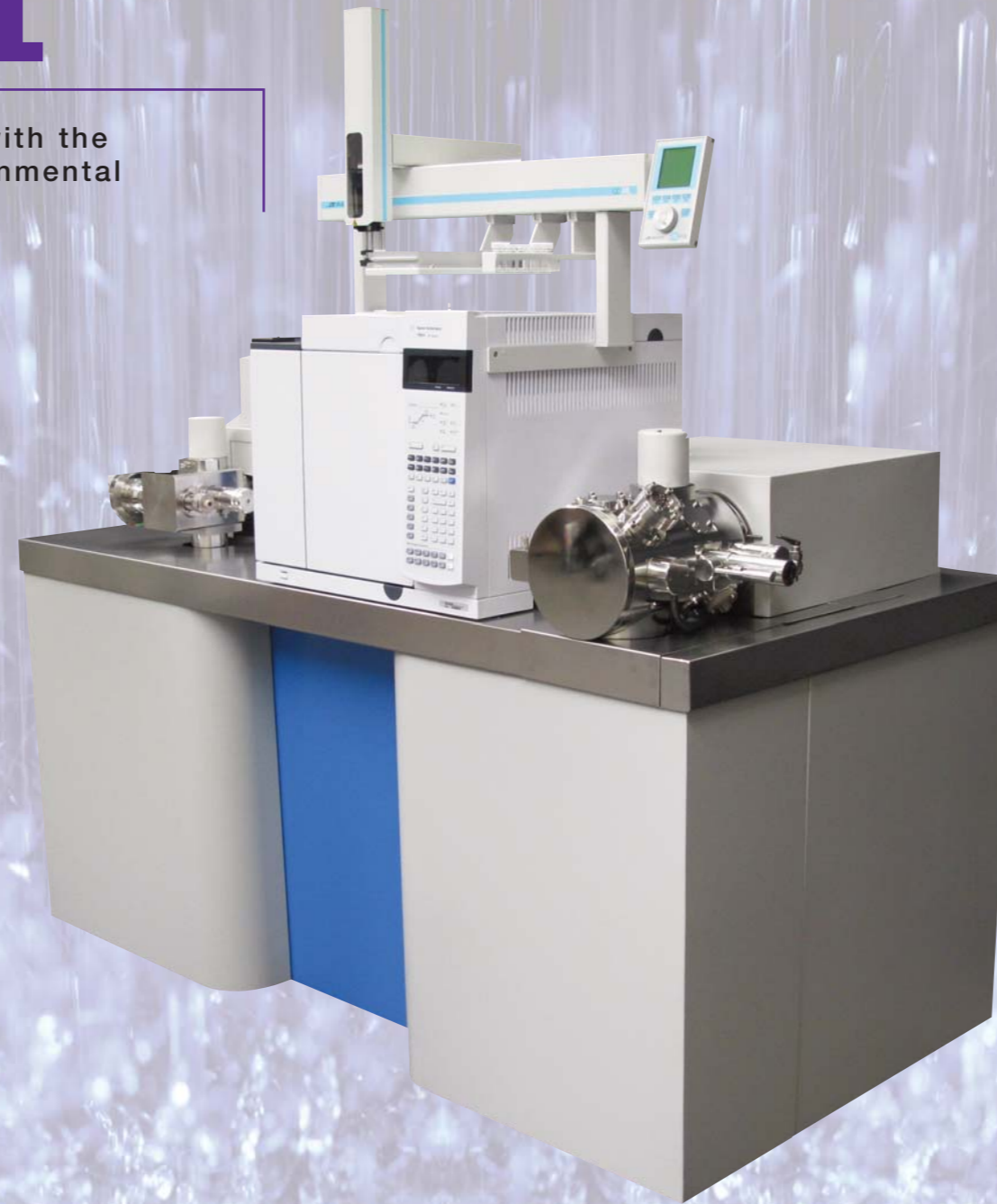


Fully-Baked Ion Optics

Unlike other mass spectrometers of its type, Autoconcept features full baking facilities along the entire flight path. This helps remove contaminants from the ion optics without the need for constant mechanical cleaning, maintaining the sensitivity and performance of the instrument at its peak.

Ion Optics Baking:

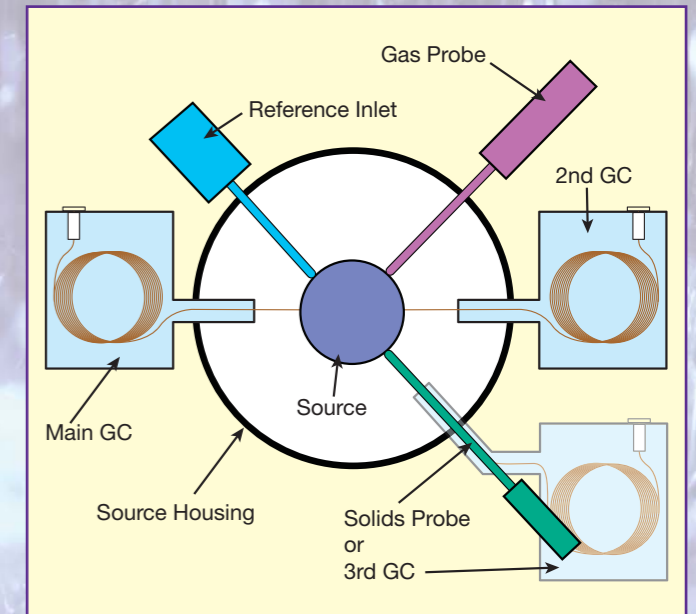
Flight path (outlined in orange) can be fully baked keeping contaminants to a minimum and performance to a maximum



Multi-technique Capabilities

Autoconcept provides much more than one analytical tool. It can be fitted with other inlets and techniques. Careful design of the source and inlet systems allows the user to operate two or even three GCs independently if required. The ability to run different GC configurations simultaneously allows rapid switching of analysis types without incurring downtime.

Other accessories such as gas probes and solid probes and a purpose built reference inlet system add to the ultimate flexibility of the Autoconcept.



Multi-GC, Multi-technique:

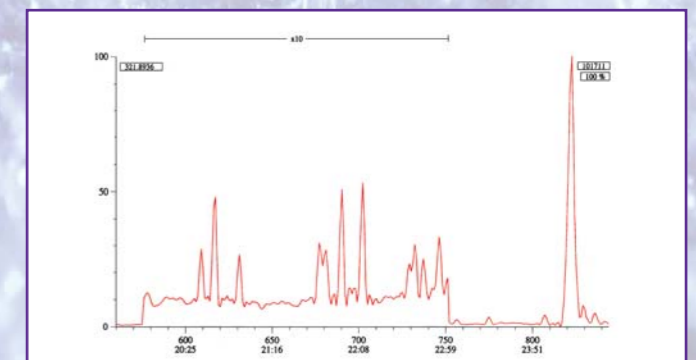
Install up to 3 GCs simultaneously and a variety of inlet options

Superior Signal-to-Noise

As well as the reduced contamination provided by the incorporated baking system, Autoconcept features an improved collector region and flight tube to further enhance detection limits.

High signal-to-noise ratios are obtained without the need to resort to ion counting and summation techniques.

Autoconcept offers this excellent sensitivity at the high resolutions required for successful dioxin and furan analysis. The combination of a source optimised for high sensitivity in electron impact mode, an analyser with the ultimate in chemical background rejection, and a low noise, high bandwidth detector system provides unmatched sensitivity at 10,000 resolution and above.



High Signal, Low Noise:

A SIM trace of 50 fg of dioxin at m/z 322 showing the noise region expanded to illustrate the high S:N ratio

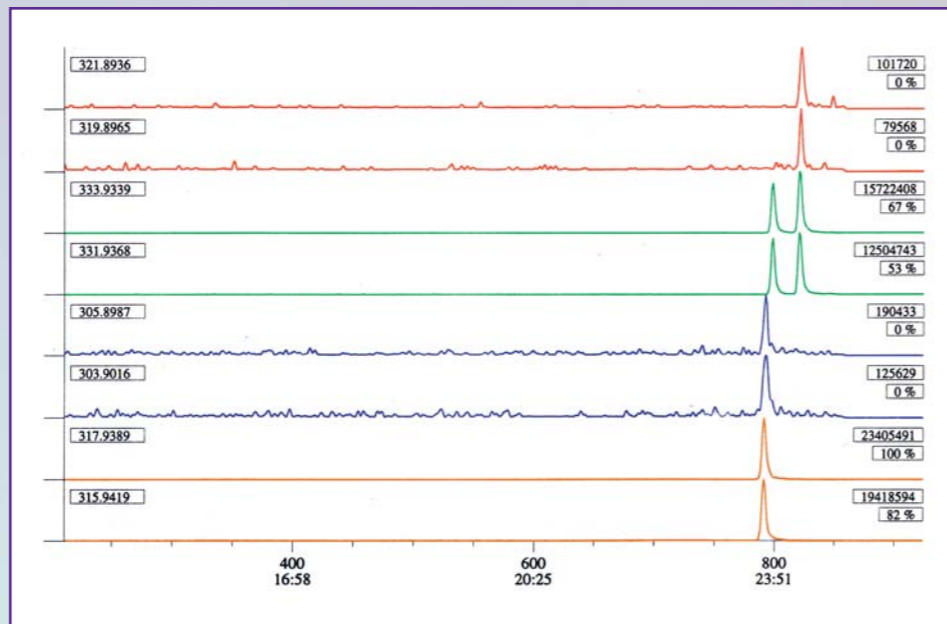
DIOXIN ANALYSIS

Autoconcept is available as a dedicated environmental high performance mass spectrometer

Autoconcept is a high performance mass spectrometer dedicated to the quantitative analysis of environmental contaminants. This type of analysis places extreme demands on instrumental performance in terms of sensitivity, stability and speed of analysis. Autoconcept from MSI fulfils these requirements for the accurate quantitation of trace level organic contaminants in environmental or other complex matrices.

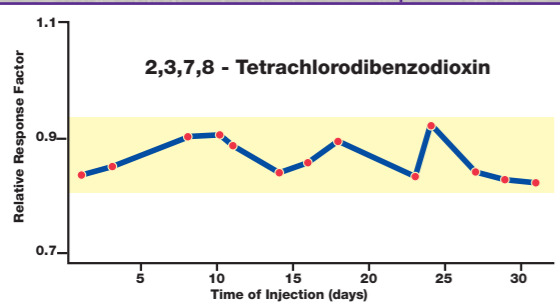
Dioxin and Furan Analysis

Protocols for environmental contaminant analysis specify high resolution mass spectrometry as the preferred detection method following high resolution gas chromatography. Only this level of instrumentation can eliminate responses from other materials present in complex matrices at sufficiently high sensitivity. Autoconcept is the instrument of choice for these dedicated analyses, in particular those with exacting requirements such as the dioxin and furan protocols specified by methods USEPA1613 and EN1948.



Dioxin Analysis:
The traces above show a typical analysis at the 50 fg level run under USEPA1613 method

Reliability:
Typical variations in response factor over an extended period of analysis show the long-term stability of the ion optics of the instrumentation



Stability

Autoconcept's ion optics involve high precision engineering yet the design has produced a very simple layout with very few focusing lenses. A minimum number of lenses provides maximum resistance to contamination effects. Autoconcept has the stability to perform analyses for days on end at optimum performance eliminating the need for time consuming recalibration. Its clip-in ion source, the area receiving the greatest contamination affront, can be changed in seconds. Maximum instrument time is spent running real samples.

Resolution

Method USEPA1613 requires a minimum of 10,000 resolution (10% valley definition). Real samples, even after clean-up and extraction, contain many other materials and require resolutions of this magnitude to provide the confidence in the results. For example:

¹³C-TCDF has an exact mass of **319.9360**

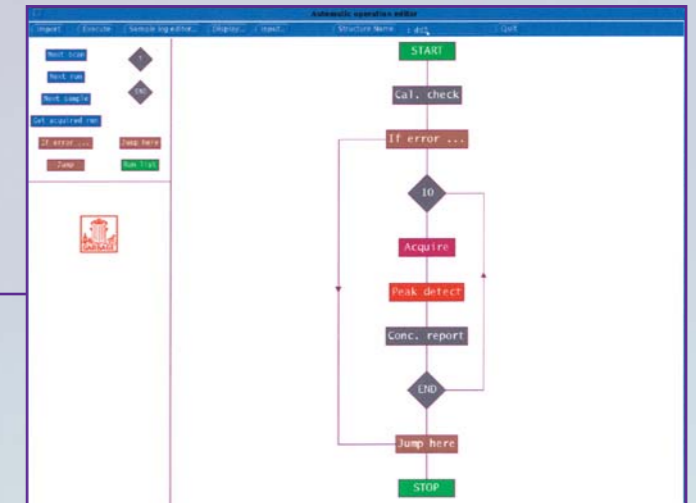
¹²C-TCDD has an exact mass of **319.8965**

The resolution required to completely resolve these would be **8100**.

Autoconcept has an ultimate resolution far in excess of this requirement which means that a resolving power of 10,000 is easily achieved routinely, time after time.

Automated Control

Autoconcept features the power of the latest MACH 3Xe control, acquisition and processing software. Autotune is a one click operation for optimised resolution and sensitivity. Complete experimental parameters can be instantly recalled for rapid sample throughput. Diagnostic controls keep instrument performance maximised. Together with GC Autosampler control, Autoconcept can be programmed to perform complete dioxin and furan analyses through the intuitive flowchart-based automated system.

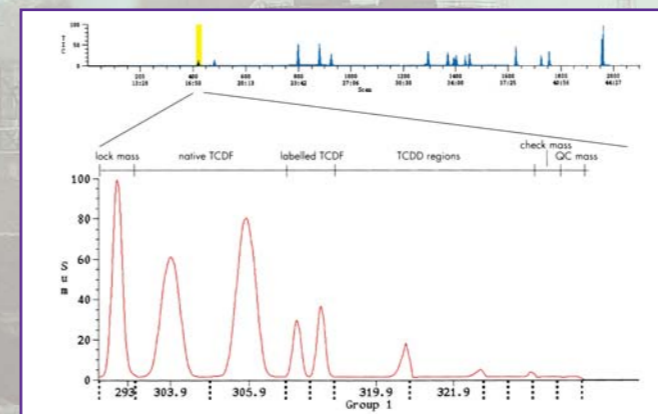


Automated Analysis:
Typical flowchart experiment created using drag-and-drop facilities

Peak Profile Analysis

Occasionally, even at high resolution, unexpected responses can be obtained. To solve this problem and to identify the cause, Autoconcept adds another tool to the analyst's armoury.

A method called **peak profiling** helps identify the origin of such responses. Instead of recording peak top responses, Autoconcept can sweep a mass region and acquire the entire peak profile, thus allowing instant recognition of any underlying interfering peaks.



Peak Profile Analysis:
The data from the individual peaks of this GC trace can be expanded to display the peak profile compositions giving absolute confidence in the results obtained

MULTI-TECHNIQUE

Autoconcept offers many additional techniques and accessories

As well as providing techniques such as accurate mass measurement and high resolution GC-MS, Autoconcept can also be configured with the following techniques and facilities:

LSIMS

Continuous Flow LSIMS

Field Desorption/Field Ionisation

Chemical Ionisation

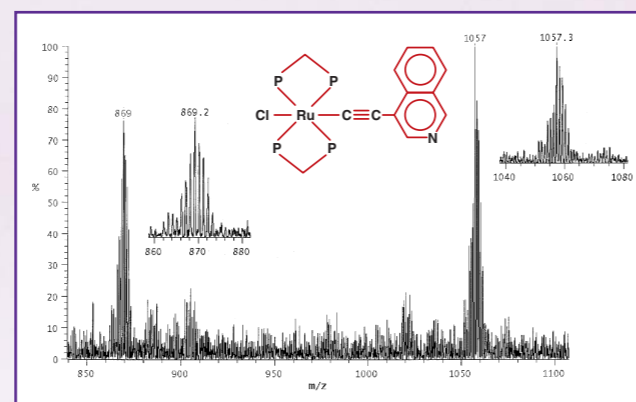
Positive and Negative Ions

Combined EI/CI

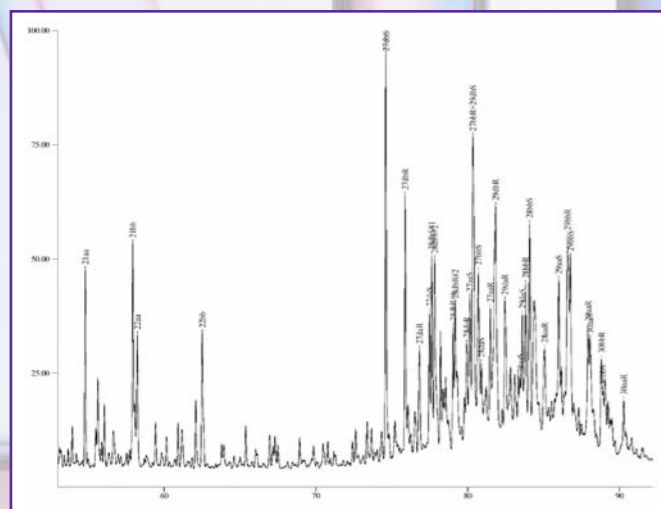
Fast Atom Bombardment

Particle Beam

Electrospray



LSIMS Analysis:
LSIMS data monitoring the synthesis of a ruthenium organometallic compound. The inserts expand the mass regions showing starting material and the resulting product.



HR-GCMS:
High resolution gas chromatography - high resolution mass spectrometry analysis of a saturated hydrocarbon fraction (C₂₁+)

Accurate Mass Measurement

The ability to specifically determine elemental composition of materials is still an essential requirement of many scientific laboratories. The better the accuracy, the higher the confidence in the result. Autoconcept can determine masses and compositions individually using the data system controlled peak matching facility for ultimate accuracy of measurement.

However, high stability combined with high precision and fast scan/digitisation speeds enable Autoconcept to calculate atomic compositions from full scans with confidence. The instrument can be set up easily and quickly using its autotuning facility, optimising both resolution and sensitivity - requirements essential for the best accuracy in mass measurements.

Measured Mass	Relative Intensity	Deviation mmu	¹² C	H	¹³ C
423.48782	3.1	-0.69	29	62	1
422.48573	9.1	0.58	30	62	0
....					
294.32760	0.5	-1.06	21	42	0
281.32088	2.6	0.05	20	41	0
280.31250	1.3	-0.50	20	40	0
267.30429	21.6	-0.88	19	39	0
266.29753	21.0	0.18	19	38	0
253.29082	2.9	1.30	18	37	0
252.28231	0.3	0.61	18	36	0
....					
85.10159	63.9	-0.13	6	13	0
84.09318	11.6	-0.72	6	12	0
71.08555	100.0	-0.53	5	11	0

Some examples of the measured masses

Squalene Analysis:
The analysis of squalene (a triterpene of molecular formula C₃₀H₆₂) performed at 10 sec/dec using a resolution of 10,000 (10% valley definition) produced these data. 10 scans were averaged to produce the full report, part of which is reproduced here



ACCESSORIES

AGHIS

The determination of oil samples in terms of their composition can provide very valuable information. By determining the amount of each class of compounds (eg paraffins, cycloparaffins, sulphur containing compounds etc) within the oil it is possible, for example, to determine the quality and also monitor any composition changes as a consequence of any chemical modifications done at a pilot plant.

Chromatographic analysis of oil samples frequently fails to provide accurate composition information. Such information can be obtained by using high resolution mass spectrometry whilst allowing the complete sample to bleed into the mass spectrometer. Scanning the mass spectrometer at a resolution of >5000 (10% valley definition) and acquiring full spectrum information with subsequent data averaging and processing with oil analysis programs, allows ready determination of composition.

The AGHIS accessory is essential for this type of analysis ensuring that the entire sample is vaporised and admitted to the mass spectrometer at a constant rate. In order to ensure that there is no sample decomposition due to the sample coming into contact with a reactive surface (eg metal), the sample introduction container is made totally from glass.



AGHIS:
The All Glass Heated Inlet System in-situ on the Autoconcept

Probe Systems

Autoconcept can be configured with a variety of inlet probe systems providing a comprehensive array of analysis options. Inlet probes include:

Solids Probe

High Temperature Solids Probe

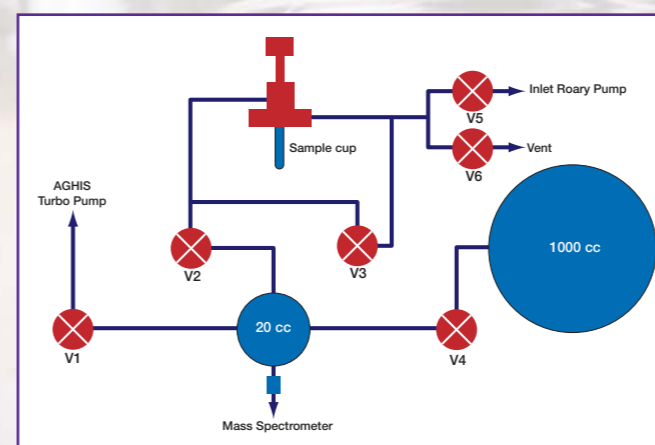
Fast Response Probe

Gas Probe

Reference Inlet System



Probe Systems:
A comprehensive range of inlet probes is available



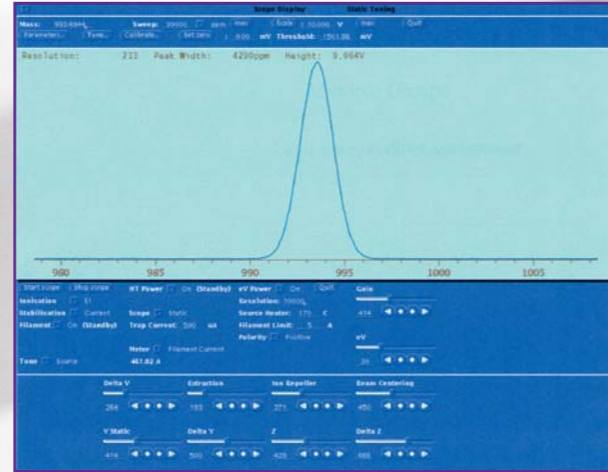
AGHIS Schematic:
Reservoir based system provides for constant flow



MACH 3Xe

High Performance Data System

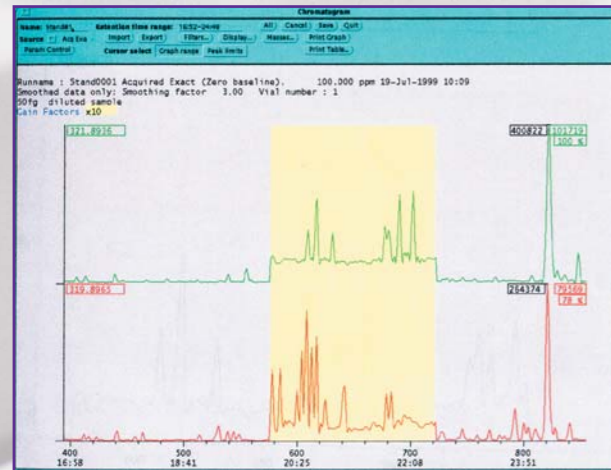
Autoconcept is equipped with the latest in high performance graphics workstations. The MACH 3Xe system runs the UNIX operating system providing some of the fastest data acquisition and processing facilities for mass spectrometry. With simplicity of set up and full automation capabilities, the combination of Autoconcept and MACH 3Xe is unbeatable for high performance environmental analysis.



SIM Experiment:
Simple to set up SIM experiments
allow storage of standard procedures

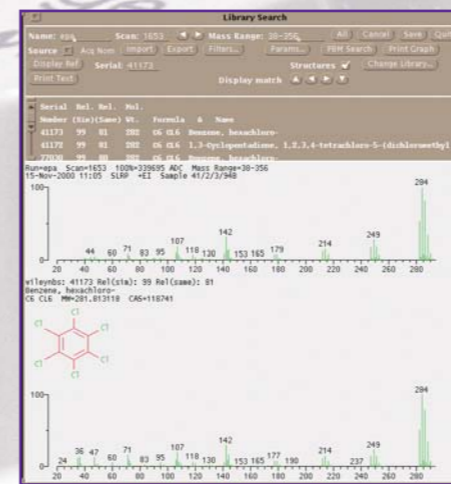
Group	Start	End	Lock Mass	Start Mass	Masses	Enabled	Fibed
1	18:00	24:30	292.9824	288.9877	11	<input checked="" type="checkbox"/>	<input type="checkbox"/>
2	24:30	29:15	330.9792	326.0146	10	<input checked="" type="checkbox"/>	<input type="checkbox"/>
3	29:15	33:20	380.9780	363.4414	8	<input checked="" type="checkbox"/>	<input type="checkbox"/>
4	33:20	38:00	430.9729	398.9014	9	<input checked="" type="checkbox"/>	<input type="checkbox"/>
5	38:00	45:00	430.9729	424.5093	8	<input checked="" type="checkbox"/>	<input type="checkbox"/>
6	coffs	coffs	coffs	coffs	0	<input type="checkbox"/>	<input type="checkbox"/>
7	coffs	coffs	coffs	coffs	0	<input type="checkbox"/>	<input type="checkbox"/>
8	coffs	coffs	coffs	coffs	0	<input type="checkbox"/>	<input type="checkbox"/>
9	coffs	coffs	coffs	coffs	0	<input type="checkbox"/>	<input type="checkbox"/>
10	coffs	coffs	coffs	coffs	0	<input type="checkbox"/>	<input type="checkbox"/>

Target Libraries:
Target compound libraries for rapid
retrieval of repeat experimental data



Autotune:
Automated tuning for optimised
resolution and sensitivity

Graphical Interface:
MACH 3Xe uses a simple graphical interface
for all control, acquisition and processing
making it one of the most intuitive data systems



Library Search:
Library search results from MACH 3Xe

Entry number	Std ref no	Type	Masses	Quantitate	To Ratio	+/	
1	2	Analyte	319.8955	<input checked="" type="checkbox"/>	2	77.00	35.00
2	3	Analyte	321.8936	<input checked="" type="checkbox"/>	0	0.00	0.00
3	4	Analyte	0.0000	<input type="checkbox"/>	0	0.00	0.00
4	5	Analyte	0.0000	<input type="checkbox"/>	0	0.00	0.00

Processing:
Comprehensive data processing
programs extract the maximum
information from each analysis





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