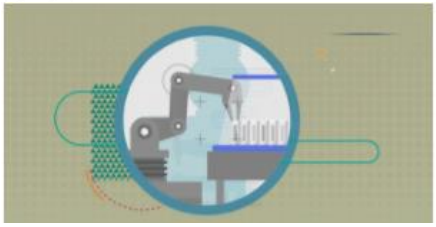
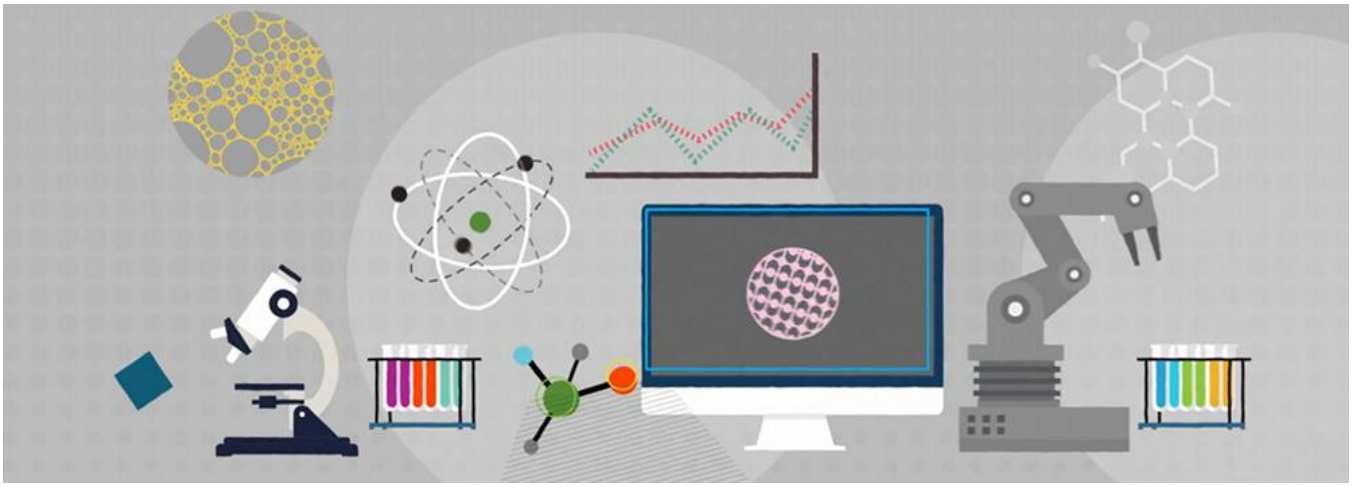


CHEMICAL ANALYSIS



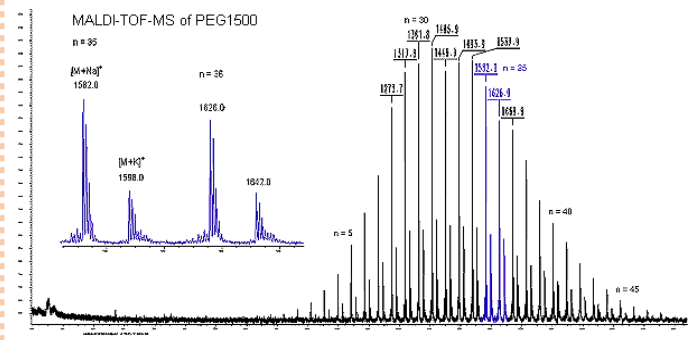
MALDI-ToF MASS SPECTROMETRY

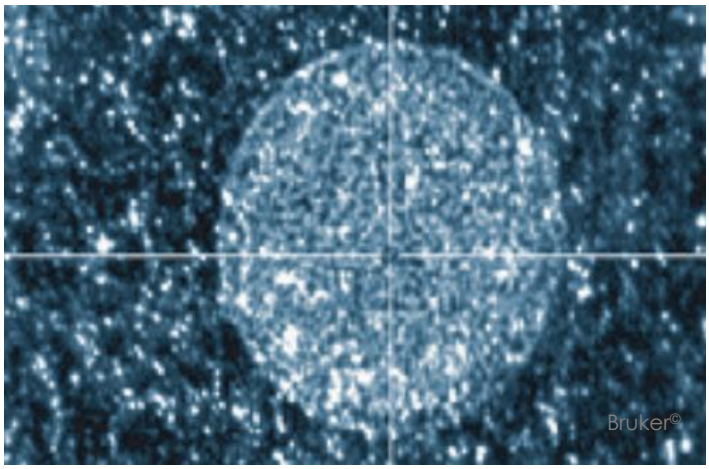
SAMPLE TYPE

Suitable for a wide range of samples from intact proteins to polymers. Matrix selection is key to obtaining good results. It is a destructive technique.

WHY USE MALDI-ToF?

- Rapid analysis of results
- Can achieve very high mass for a MS system
- Simple sample preparation
- Uses approx. 2 mg of sample per target spot
- MS/MS measurement





Bruker Smartbeam technology provides the maximum MS signal with minimum sample consumption enabling maximum data extraction from precious samples.

WHAT IS IT?

Matrix Assisted Laser Desorption Ionisation – Time of Flight Mass Spectrometry or MALDI-ToF MS.

A mass spectrometer coupled to a powerful laser capable of measuring high mass ranges that are not possible with a traditional ESI/APCI source.

The sample is mixed with an excitation matrix and recrystallized onto a target plate. The plate is introduced into an evacuated chamber.

AutoFlex©

SPECIFICATION / ATTACHMENTS

Bruker AutoFlex

- MALDI Perpetual Ion Source
- Pulsed Ion Extraction
- Bruker Smartbeam technology
- MS/MS capability
- ToF analyser for linear and reflectron measurements
- Ground Steel, Anchor Chip and Polished Steel target plates

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.bruker.com

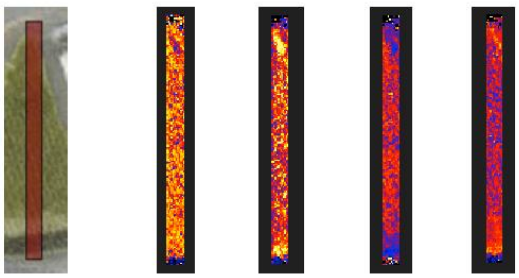
IMAGING MASS SPECTROMETRY

SAMPLE TYPE

Imaging mass spectrometry is a mapping technique used on samples where the spatial resolution of differing masses is of key importance.

WHY USE IMAGING MASS SPECTROMETRY?

- Results are resolved in spatial coordinates in addition to masses
- Can achieve very high mass for a MS system
- Easy sample preparation
- Rough surfaces can be analysed

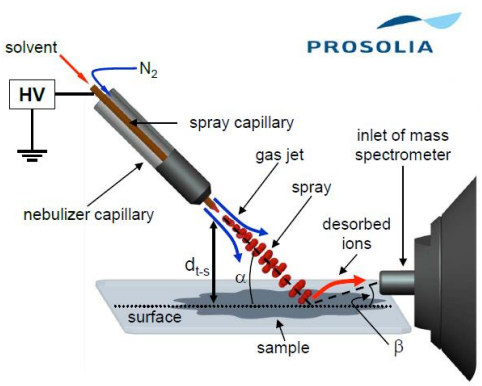


Fabric heatmap

Desorption

Electro**S**pray

Ionisation



WHAT IS IT?

A mass spectrometer coupled to a powerful laser or DESI source.

A laser or a solvent mix is directed to the surface of a plate which contains the sample. The sample is moved according to a pre-programmed raster and mass spectra are taken at each point.

Post processing of the continuous mass spectra allows the spatial resolution to be deconvoluted and an image of the differing masses extracted for each raster point.

Synapt G2-Si©

SPECIFICATION / ATTACHMENTS

Waters Synapt G2-Si mass spectrometer

- MALDI Laser source
- DESI source gives atmospheric pressure analysis with minimal preparation
- HDI Software for programming and post processing image manipulation
- Modes can be switched in roughly 2 hours

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

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Supplier website: www.waters.com

SUPERCRITICAL FLUID CHROMATOGRAPHY (SFC)

WHY SFC?

SFC allows the user to precisely vary the mobile phase strength, pressure and temperature to fine-tune the resolving power and selectivity of the system to separate, detect and quantify structural analogs, isomers, enantiomers and diastereomers.

This system is configured with a high pressure flow cell photo diode array detector (PDA) for sample detection and quantification.

Waters©

WHAT IS IT?

SFC is a chromatographic technique which uses the inexpensive and non-toxic compressed liquid CO_2 as a primary mobile phase to separate complicated mixtures.

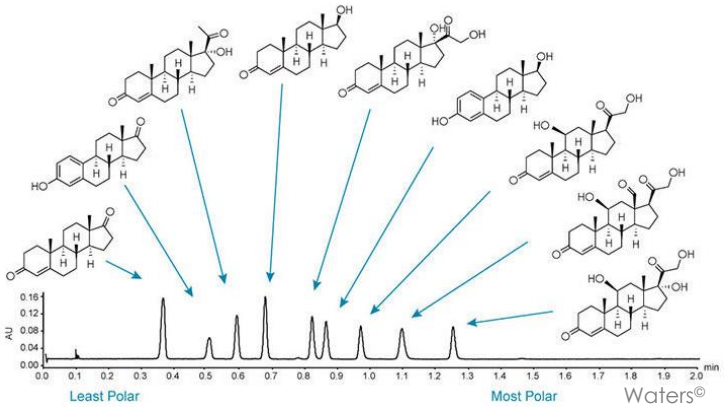
SFC is a relatively new technique which can be classed as convergence chromatography as it combines the ease-of-use of reversed phase liquid chromatography with the separation power of normal phase chromatography.

Waters©

MASS SPECTROMETRY ANALYSIS

This system can be coupled to either a Triple Quadrupole Detector (TQD) or Quadrupole Time of Flight (QToF) mass spectrometer for improved detection identification.

The combined use of a mass spectrometer for peak identification, photodiode array detection for quantification and the ability to fine tune the method parameters makes this the ideal choice for complex mixture analysis.



Waters©

SPECIFICATION / ATTACHMENTS

Waters UPC² SFC

- Operating flow rate: 0.01 to 4 mL/min
- Maximum pressure: 6000 psi (413 bar)
- Injection volume: 0.1 to 50µL
- Sample Temperature control: 4 to 40°C
- Variety of columns available

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.waters.com

XEVO TRIPLE QUADRUPOLE DETECTOR (TQD) MASS SPECTROMETER

WHY USE A TQD?

The increased selectivity, improved signal to noise ratio, lower limits of quantitation and wider linear range make this an excellent method for challenging samples.

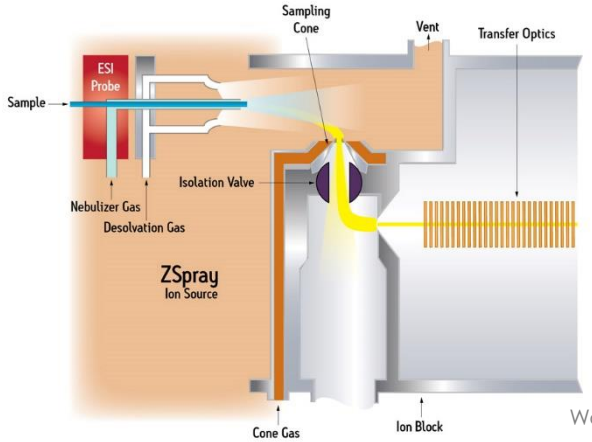
The TQD is connected to a quaternary liquid chromatography system enabling both isocratic and gradient elution or a Waters UPC^2 SFC system for the separation of complex mixtures prior to mass spectrometry.

Waters©

ZSPRAY IONIZATION SOURCE

A range of ionization methods are available:

- **ESI:** Electrospray Ionisation
- **APCI:** Atmospheric Pressure Chemical Ionisation
- **ESCi®:** Dual ESI and APCI

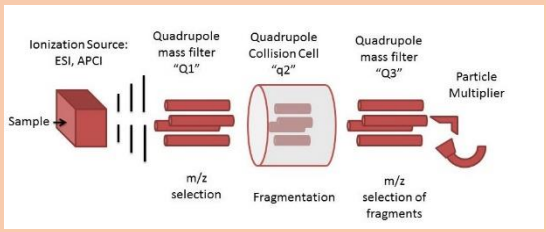


Waters©

WHAT IS IT?

A triple quadrupole is a mass spectrometer in which the first and third quadrupoles act as mass filters and the second quadrupole fragments the analyte within a collision cell.

Schematic of a typical triple quadrupole mass spectrometer:



Wikipedia

SPECIFICATION / ATTACHMENTS

- Waters Xevo TQD
- Mass Range: 2 to 2048 m/z
- Scan Speed: Up to 10,000 Da/s
- Mass Stability: Mass drift < 0.1Da (24h)
- Up to 16,384 MRM channels
- ESI, APCI and ESCi® ionization sources
- Acquisition modes:
- Full Scan MS
- Product ion scan
- Precursor ion scan
- Multiple reaction monitoring
- Autosampler: 96 x 2 mL vials
- Column temperatures: 20 to 65°C

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.waters.com

XEVO G2- QUADRUPOLE TIME-OF-FLIGHT(QToF) MASS SPECTROMETER

WHY USE A QToF?

QToF is a high resolution mass spectrometer with the ability to measure accurate mass to charge ratios (m/z) with four decimal places providing unparalleled substance identification.

The ability to perform MS/MS analysis in which the quadrupole selects a specific precursor ion which is then fragmented in a collision cell and the fragments detected in the ToF allow structural identification to be performed.

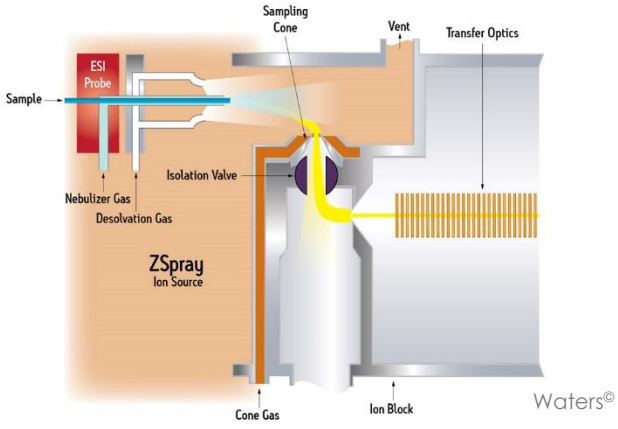
The QToF is connected to a quaternary liquid chromatography system enabling both isocratic and gradient elution or a Waters UPC^2 SFC system for the separation of complex mixtures prior to mass spectrometry.

Waters©

ZSPRAY IONIZATION SOURCE

A range of ionization methods are available:

- **ESI:** Electrospray Ionisation
- **APCI:** Atmospheric Pressure Chemical Ionisation
- **ESCi®:** Dual ESI and APCI



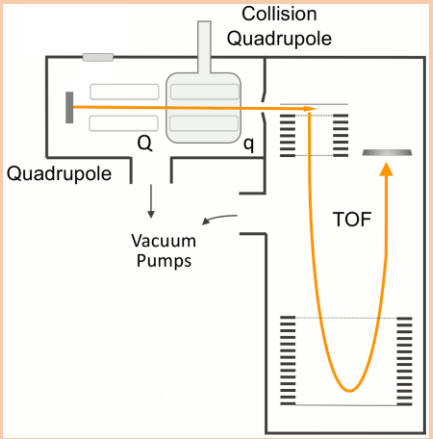
Waters©

WHAT IS IT?

A Quadrupole Time-of-Flight (QToF) mass spectrometer combines the ion selection properties of a quadrupole with the high mass resolution and accuracy of a ToF in a single system.

The mass to charge ratio (m/z) of an ion are determined by measuring the time of flight of the accelerated ions by an electric field of known strength in a known distance.

The heavier ions travel slower than the lighter ions.



SPECIFICATION / ATTACHMENTS

- Waters Xevo G2-XS QToF
- Mass range: 20-100,000 m/z
- Positive and negative detection modes
- Mass accuracy: 1ppm with up to 40,000 FWHM mass resolution
- ACQUITY LC system with flow rate: 0.01 to 2mL in 0.001mL increments
- 96 x 2mL vials

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.waters.com

PREPARATIVE HPLC

WHAT IS IT?

The Agilent preparative HPLC has an automated fraction collector which enables collection by UV signal or mass based detection depending on your sample characteristics. Two preparative pumps are each capable of delivering up to 100 mL/min at 400 bar pressure enabling large bore semi-prep columns to be used. The ChemStation software package provides full data collection and analysis including automated and manual integration of peaks, report generation and mass ion characterisation. A range of general HPLC columns are provided.

SAMPLE TYPE

- A variety of soluble samples in solution
- Injection of up to 5 mL of sample
- Separation of organic samples
- Capability to plug difficult to dissolve samples

Agilent HPLC System©

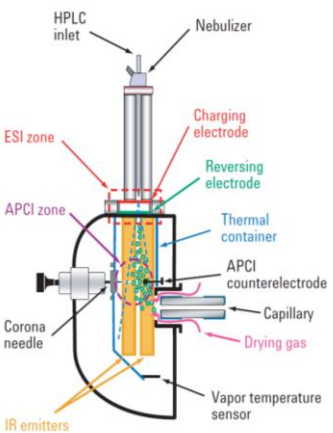
SPECIFICATION / ATTACHMENTS

- Diode Array Detector 190-600 nm
- Multimode APCI and ESI source
- M/Z ratio up to 2000
- Range of columns
- Sample loops of 50 µl to 5000 µL

WHY USE the Preparative HPLC?

- Separation of samples based on mass or absorbance
- Purification of materials based on mass or absorbance
- Analysis of difficult to separate samples

Overview of the Multimode Source



1. LC eluent and nebulizing gas enter the grounded nebulizer
2. A charged aerosol is generated in the ESI zone; spray direction is orthogonal to capillary axis
3. The aerosol is dried by infrared emitters and heated drying gas, producing ions by ESI
4. The aerosol and ions flow with the nebulizing gas from the ESI zone to the APCI zone
5. Infrared emitters completely vaporize the solvent and analyte in the APCI zone
6. A corona is produced between the corona needle and APCI counterelectrode, ionizing the solvent
7. Ionized solvent transfers charge to the analyte molecules, producing analyte ions
8. ESI ions pass behind a separator (not shown) that screens them from the APCI corona
9. Power to the infrared emitters is controlled by the vapor temperature sensor, maintaining constant temperature
10. ESI and APCI ions simultaneously enter the capillary

Columns

- Zorbax SB-CN 2.1 x 150 mm 1.8 µm
- Zorbax SB-C18 4.6 x 50 mm 5 µm
- Zorbax SB-C18 9.4 x 250 mm 5 µm
- Zorbax SB-C18 4.6 x 250 mm 5 µm
- Zorbax SB-CN 4.6 x 250 mm 5 µm
- Poroshell 120 EC-C18 4.6 x 100 mm 4 µm
- Zorbax SB-C18 9.4 x 50 mm 5 µm
- Zorbax SB-C8 2.1 x 50 mm 5 µm
- Zorbax Eclipse Plus C18 4.6 x 100 mm 3.5 µm

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.agilent.com

GAS CHROMATOGRAPHY - MASS SPECTROMETRY (GC-MS)

WHY USE GC-MS?

GC-MS is an analytical technique by which complex mixtures of chemicals may be separated, identified and quantified in the gaseous phase.

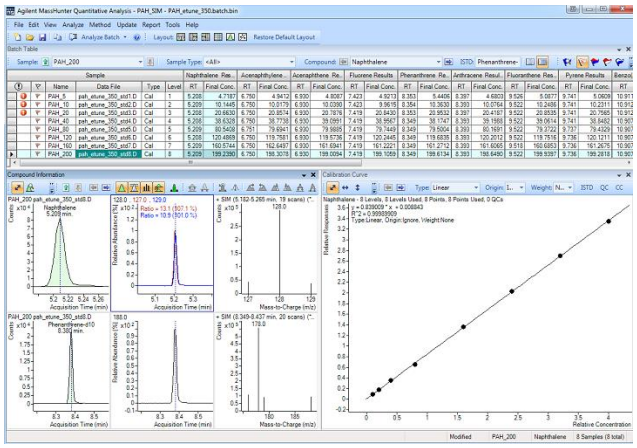
Agilent©

WHAT IS IT?

The Agilent 7890B GC is the world's most widely used GC system. It features accurate temperature controls (+4°C to 450°C) and precise injection systems, plus enhanced Electronic Pneumatic Control modules for best retention times.

This is coupled with the new Agilent 5977B EI High Efficiency Source (HES) MSD. The HES maximises the number of ions that are created and transferred out of the source body into the single quadrupole analyser, resulting in improved sensitivity (10x) and detection limits as low as 1.5fg instrument detection limit.

DATA ANALYSIS



This is a easy to learn software platform which handles all your qualitative and quantitative analysis tasks. Typical tasks performed by MassHunter includes identification, characterisation and quantitation of unknown substances or metabolite identification.

SPECIFICATION / ATTACHMENTS

- Single filament Thermal Conductivity Detector (TCD) provides a stable baseline with a minimal of signal drift.
- Auto-ranging Flame Ionisation Detector (FID) provides the ability to detect and quantitate from parts per billion to parts per thousand in a single injection.
- Auto sampler provides the user with the ability to perform liquid injections and supports syringe volumes from 1.2 µL to 10,000 µL. It also provides the user with the ability to perform Solid Phase Micro-Extraction (SPME).
- NIST 2014 MS library bundle includes 243k spectra with names, chemical structures, and retention indices. Includes MS/MS spectra library, NIST search and AMDIS programs.

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.Agilent.com

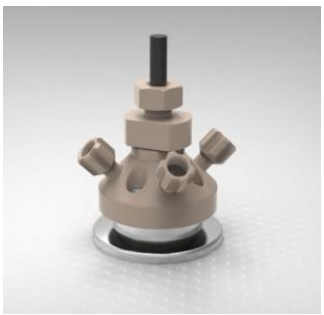
GAS CHROMATOGRAPHY-DIFFERENTIAL ELECTROCHEMICAL MASS SPECTROMETRY (GC-DEMS)

WHY USE GC-DEMS?

GC-DEMS is an analytical technique that allows the separation and *in situ* mass resolved determination of gaseous or volatile reactants, reaction intermediates and products from electrochemical reactions.

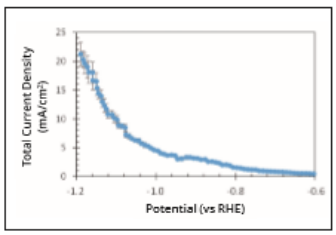
Hiden's quadrupole mass spectrometer systems address a broad application range in: vacuum, gas, plasma and surface science.

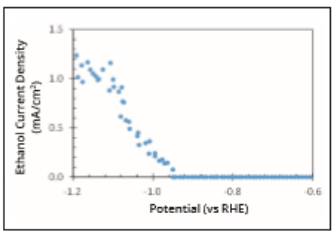
Hiden©

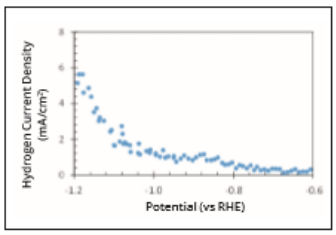


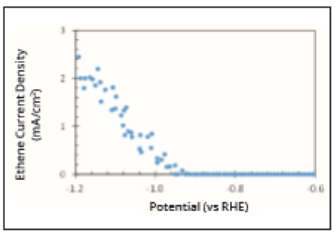
A Hiden Analytical DEMS Cell

Hiden©









WHAT IS IT?

The Agilent 7890B GC is the world's most widely used GC system. It features accurate temperature controls (+4°C to 450°C) and precise injection systems, plus enhanced Electronic Pneumatic Control modules for best retention times.

This is coupled with a Hiden Analytical HPR-40 DEMS, which scans the electrochemical potential and applies mass spectrometry to analyse the products. Typical scanning speeds are around 1 mV/s with a typical scanning range of 0 to -1.5V.

SPECIFICATION / ATTACHMENTS

- Type A DEMS cell for materials/catalysis studies.
- Type B DEMS cell for electrochemical reaction studies.
- Mass ranges: 1-200 amu
- Sensitivity: 100% to 100 ppb subject to spectral interference
- Speed: up to 650 measurements/second
- Response time: <1 s (dependant on flow rate)
- Detector: Dual Faraday / Electron Multiplier

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

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Supplier website: www.Hiden.com

VISCOTEK TDA302 GPC x 2

SAMPLE TYPE

Polymers of any weight range can be used in the GPC. They need to be solubilised in an appropriate solvent before use.

Polymers can be of any class as we have two instruments. One is set up for organic solvent analysis (THF/Toluene) and another for water analysis.

WHAT IS IT?

The Visctotek TDA302 performs reliable measurements of the molecular weight distribution of polymers.

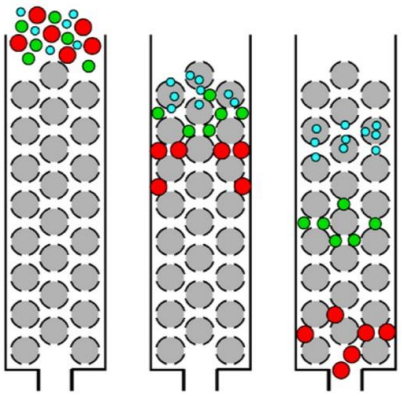
Using an appropriate column molecular weights of a large range of polymer chain lengths can be analysed.

Malvern©

HOW GPC WORKS

GPC works on a size exclusion principle (SEC)

A column is packed with materials of defined porosity. Larger polymers pass through the column faster and are eluted first. By using polymers of a known molecular weight the column can be calibrated and the molecular weight of an unknown polymer can be deduced



SPECIFICATION / ATTACHMENTS

- 2 systems available for sample submission – one organic and one water
- Range of columns for broad and narrow Mw work
- Set up for water soluble polymers
- Organic solvent soluble polymers by request
- Quadruple detection – Refractive Index, Differential pressure, Internal pressure, Ultra-Violet

TASKS AND APPLICATIONS

- Analysis of M_p, M_n, M_z, M_w and PDI of polymers
- Qualitative analysis of bimodal polymers
- Elucidation of the total percent of polymerisation

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.Malvern.com

OMNISEC RESOLVE/REVEAL GPC

SAMPLE TYPE

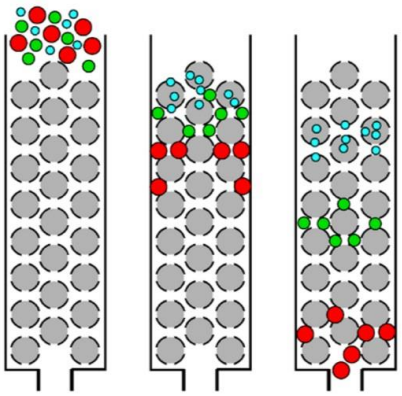
Polymers of any weight range can be used in the GPC. They need to be solubilised in an appropriate solvent before use.

Polymers can be of any class. The system is set up for the analysis of polymers soluble in water but can be changed to the organic phase by request.

HOW THE GPC WORKS

GPC works on a size exclusion principle (SEC)

A column is packed with materials of defined porosity. Larger polymers pass through the column faster and are eluted first. By using polymers of a known molecular weight the column can be calibrated and the molecular weight of an unknown polymer can be deduced.



TASKS AND APPLICATIONS

- Analysis of M_p, M_n, M_z, M_w and PDI of polymers
- Qualitative analysis of bimodal polymers
- Elucidation of the total percent of polymerisation

WHAT IS IT?

The Omnisec Resolve/Reveal performs reliable measurements of the molecular weight distribution of polymers.

Using an appropriate column molecular weights of a large range of polymer chain lengths can be analysed.

Malvern©

SPECIFICATION / ATTACHMENTS

- Single system for insoluble polymers or research work
- Range of columns for broad and narrow Mw work
- Set up for water soluble polymers
- Organic solvent soluble polymers by request
- Triple detection – Refractive Index, Differential pressure, Internal pressure
- 10x sensitivity over the TDA302

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.Malvern.com

CONFOCAL RAMAN SPECTROSCOPY

SAMPLE TYPE

Raman can be used for a wide variety of samples including: inorganics, organics and biological samples, in general the only sample types not suitable are mainly metals and their alloys.

WHY USE RAMAN?

- Detailed structural analysis/characterisation
- Rapid speed
- Non-invasive/non-destructive
- Little to no sample preparation
- Confocal analysis, 3D spatial resolution
- True *in situ* and *in vitro* analysis
- Live tracking

RAMAN Vs IR

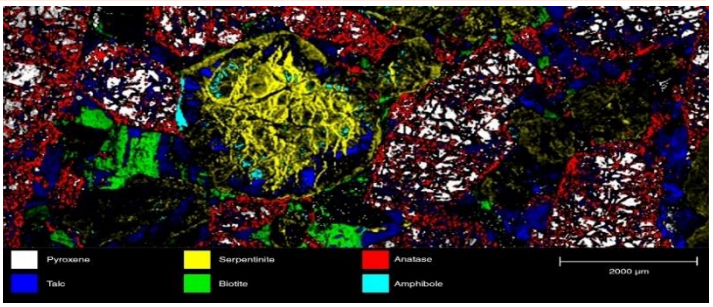
Raman spectroscopy is based on a change in polarizability, whereas IR is when a molecule undergoes a dipole change. For example, symmetrical molecules do not have IR absorption, but will produce Raman scattering.

Imaging

Analogous to taking actual photographs, where spectral values are collected simultaneously from the area of interest. A single image is collected rapidly.

Mapping

A spectrum is collected at each position of the sample, either point-by-point or in a line focus.



StreamLine image of igneous rock©

WHAT IS IT?

A spectroscopic technique that uses monochromatic light and inelastic scattering to observe vibrational and rotational modes in a sample.

A laser interacts with excitations in a system, which result in energy shifts, which are then used to give information about the vibrational modes.

Results are usually generated in a spectral format and the Renishaw system can also provide imaging and mapping capabilities.

Qontor image©

SPECIFICATION / ATTACHMENTS

Renishaw InVia™ Qontor®

- 532 nm and 785 nm laser
- 10x, 50x and 100x standard objectives
- 100x oil immersion and 63x water immersion
- WiRE 4.4 software
- Hot and cold stage
- Macro sampling kit

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.renishaw.com

FLUORESCENCE LIFETIME SPECTROSCOPY (FLS)

SAMPLE TYPE

Fluorescence lifetime spectroscopy (FLS) is used to measure the excitation and emission spectra of liquid samples within cuvettes, multiwell plates or solid samples.

FLS has a very low limit of detection allowing very weak (<100 fM) samples to be analysed.

WHY USE FLUORESCENCE LIFETIME SPECTROSCOPY?

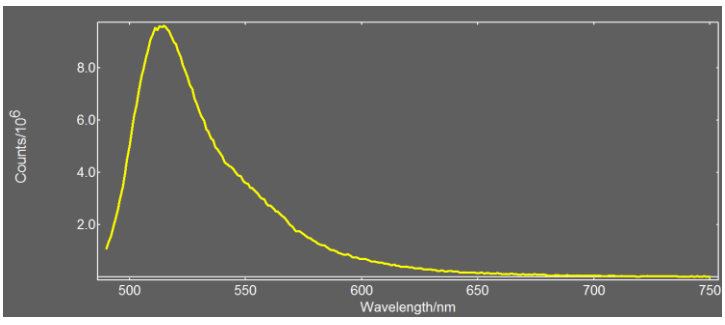
- Provide quantitative information
- Rapid speed
- Non-invasive/non-destructive
- Little to no sample preparation
- Extremely low detection limits

TIME-CORRELATED SINGLE PHOTON COUNTING (TCSPC)

TCSPC involves the excitation of your sample with a specific pulsed diode laser or LED source and measuring the time taken for each photon to decay to the ground state (typically 100 ps-50 µs).

The following laser/LED excitation sources are available:

310,375,445,475,560 and 640 nm



WHAT IS IT?

A spectroscopic technique which involves excitation of your sample at a specific wavelength and the measurement of emission of this energy as fluorescence as the sample returns to the ground state.

This FLS1000 instrument can also be configured to perform Time-Correlated Single Photon Counting (TCSPC) to measurement the lifetime of fluorescence.

FLS 1000©

SPECIFICATION / ATTACHMENTS

Edinburgh Instruments FLS1000

- 200-870 nm wavelength range
- Signal to noise ratio >25,000:1
- Rapid measurements <30 s
- Sample holders for liquids, films and solids
- Full Fluoracle software package for excitation, emission, synchronous and TCSPC measurements.
- Advance FAST software available for detailed TCSPC analysis

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

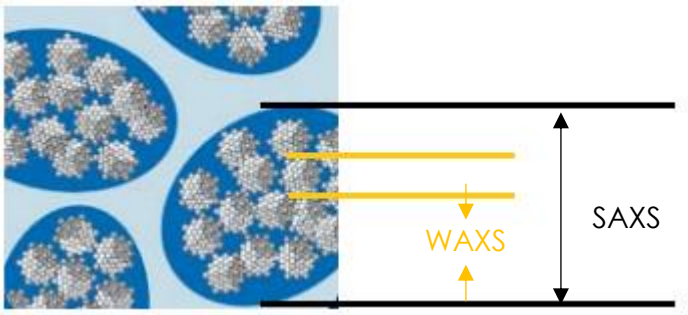
0151 795 7100

Supplier website: www.edinst.com

SMALL ANGLE X-RAY SCATTERING (SAXS)

SAMPLE TYPE

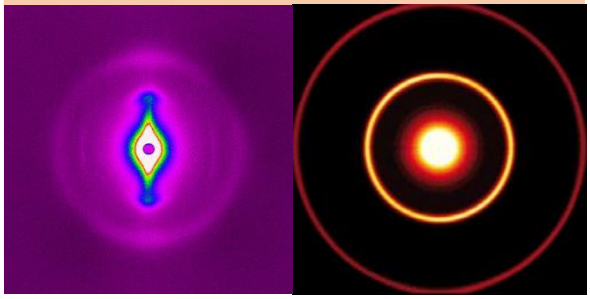
The Bruker Nanostar system is capable of characterising the nanostructures of non-crystalline materials, both solid and liquid samples, ranging from 1 nm to roughly 125 nm.



SAXS can give you information about the shape and size distribution of your particles, as well as how far apart they sit in space.

WHAT IS IT?

Small Angle X-ray Scattering is a phenomenon caused by particles embedded in a matrix of different electron density. If the particle size ranges from 1 nm to 100 nm, the scattering angle lies within the range of 0° to 5°. The smaller the particles, the wider the scattering angles.



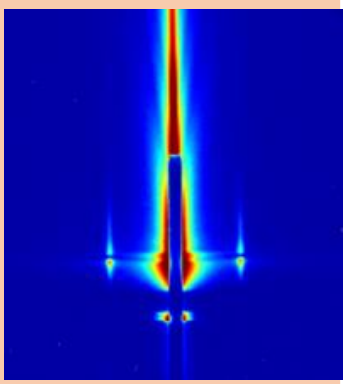
Bruker©

WHY USE SAXS?

- Rapid measurement speed due to gallium liquid anode
- Non-invasive/non-destructive
- Little to no sample preparation
- Allows *in-vivo* and *in-situ* measurement

GISAXS

GISAXS allows you to probe the surface of your samples by detecting the reflectance of the X-ray beam. This enables the study of material deposited on surfaces, thin layers of nanomaterials or nanostructured particles.



SPECIFICATION / ATTACHMENTS

- Motorised X-Y stage
- Detector to sample distance from 11.5 mm to 1070 mm covering SAXS and WAXS
- GISAXS sample stage
- Heating/cooling stage
- Measurement in gas atmosphere

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.bruker.com

INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS)

WHY ICP-MS?

For nearly 30 years, ICP-MS has been gaining favour with laboratories for performing trace metal and elemental analysis with detection limits at or below the part per billion (ppb) level.

An analytical working range of >10 orders of magnitude is available which is unsurpassed by any other technique.

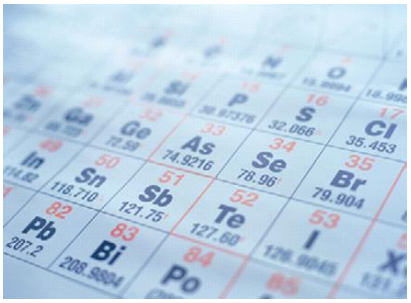
Perkin Elmer©

ANALYSIS

Semi-quantitative: Provides a fingerprint of the elements present in a sample and the approximate concentrations.

Quantitative: Accurately determines how much of a specific element is in the material analysed.

Isotopic analysis: Specific isotopes of an element can be measured and their ratio determined.



WHAT IS IT?

ICP-MS is an analytical technique primarily used for elemental determination.

The sample is introduced into the ICP plasma via nebuliser. Samples are typically solutions using an auto-sampler or solid samples using a laser ablation technique.

A high temperature inductively coupled plasma source converts atoms in a sample to ions and these are directed into a mass spectrometer.

A quadrupole mass spectrometer separates the ion by their mass to charge ratio (m/z).

SPECIFICATION / ATTACHMENTS

- The NexION 2000 has the fastest data acquisition speed (100,000 points per second) available and is best equipped for nanoparticle determinations.
- A mass range of 1-285amu is available with the quadrupole MS.
- The NexION 2000 can be ran in either standard, collision or reaction mode depending on interences.
- This system is the only ICP-MS available that can run pure ammonia for complete and targeted interference removal.

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website:
www.perkinelmer.co.uk

TESCAN S8000G FOCUSED ION BEAM (FIB)/SCANNING ELECTRON MICROSCOPE (SEM) EQUPPED WITH A CRYO-STAGE, ENERGY DISPERIVE SPECTROSCOPY (EDS) AND WAVELENGTH DISPERSIVE SPECTROSCOPY (WDS)

WHY FIB/SEM?

The SEM is used to study solid materials and liquids (using the cryo-stage). The spatial resolution is ~1nm. EDS and WDS are used to determine elemental composition, and FIB to obtain 3D reconstructions and prepare cross-sections and TEM lamellae.

Figure 1: Tescan S8000G (Tescan©)

Cryo-SEM and Cryo-FIB

The cryo-stage is the Quorum PP3010, and is used to cool liquid specimens to the temperature of liquid nitrogen. These are can be studied in the SEM (Figure 2), or milled using the FIB to reveal internal porosity etc.

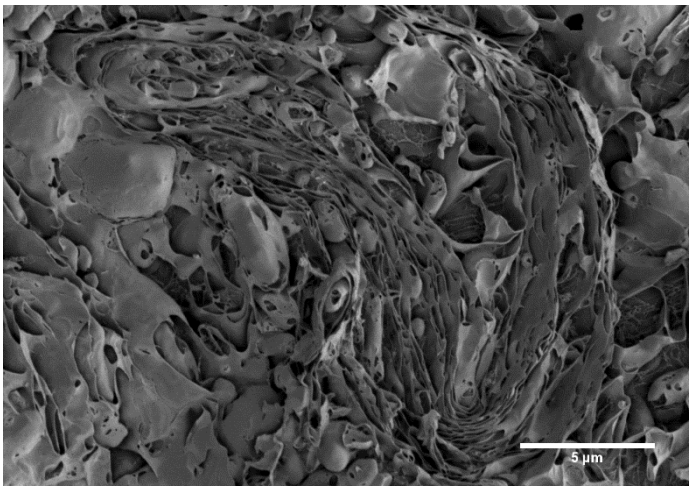


Figure 2: Hair conditioner studied using Cryo-SEM (sample Courtesy of Unilever)

WHAT IS IT?

The Tescan S8000G FIB/SEM has a thermal Field Emission Gun (FEG) capable of producing 400 nA of beam current. Images are obtained using in-chamber and in-column secondary electron (SE) and back-scattered electron (BSE) detectors. The instrument has a gallium ion column capable of producing 100 nA beam current.

The analysis suite is provided by Oxford Instruments, and is comprised of EDS and WDS systems. Data collection is fast using EDS, but some elements overlap (Figure 3). These can easily deconvoluted using WDS (also shown in Figure 3).

Both the EDS and WDS are calibrated so that analysis can be fully quantitative.

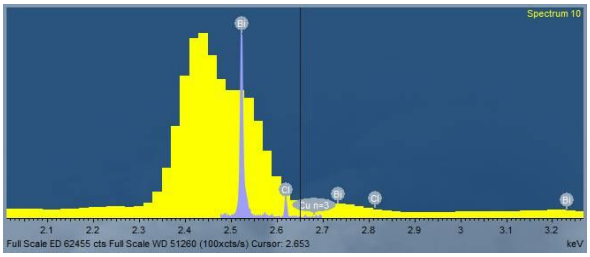


Figure 3: Synthesized material containing Bismuth and Chlorine – EDS spectrum (yellow), and WDS spectrum (purple)

SPECIFICATION / ATTACHMENTS

Please contact the MIF Technical team using the details below for further instrument details.

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

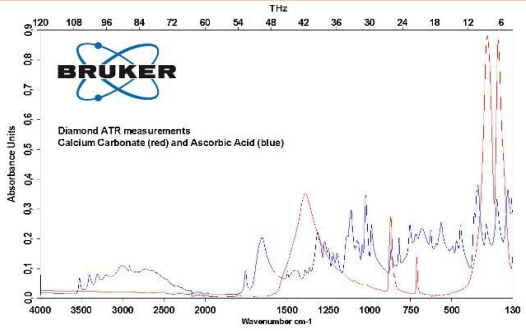
Supplier website: www.tescan.com

FT-IR SPECTROSCOPY

WHY USE FT-IR?

Fourier-transform infrared (FT-IR) is used by chemists to determine functional groups within molecules, mainly in organic and polymeric samples.

The applications of FT-IR are almost limitless as it can provide both qualitative and semi-quantitative analysis in areas ranging from QA/QC testing to investigative studies.



DIAMOND Vs GERMANIUM

The germanium crystal has a higher RF value (4) compared to the diamond crystal (2.4). This means that it has a major advantages for analysing very dark samples, but the disadvantage that the crystal is very soft compared to the diamond. The germanium crystal can therefore not be used for sharp samples such as polymers and is more suited to carbon black etc.

DETECTORS

The FT-IR has two different detectors, the Deuterated Triglycine Sulfate (DTGS) and the Mercury Cadmium Telluride (MTC).

DTGS	MTC
Room temperature	Cooled using liquid nitrogen
Standard detector	1000x more sensitive
Scanner velocity: ≤10kHz	Scanner velocity: 20kHz

WHAT IS IT?

Infrared (IR) radiation is passed through a sample, some of this radiation will be absorbed and some will be transmitted by the sample, the extend of which is sample dependent. Each sample produces a spectrum known as the 'molecular fingerprint' which is interpreted and used to provide structural information about the sample.

FT-IR is used widely in both industry, R&D and academia due to its speed and precision for structural information.

VERTEX 70©

SPECIFICATION / ATTACHMENTS

- Vertex 70 FT-IR Spectrometer
- DTGS and MTC detector
- OPUS software
- Diamond crystal
- Germanium crystal
- Transmission accessory
- 96 well plate reader

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.bruker.com

UV/Vis/NIR SPECTROSCOPY

SAMPLE TYPE

UV/Vis/NIR spectroscopy characterises a wide variety of samples: from liquid samples in cuvettes, to translucent thin films, and even opaque solids. The Agilent Cary 5000 can measure the absorbance of light (up to 8.0 Abs) between 175-3300 nm. The internal diffuse reflectance accessory (DRA) can be used to measure the reflectance.

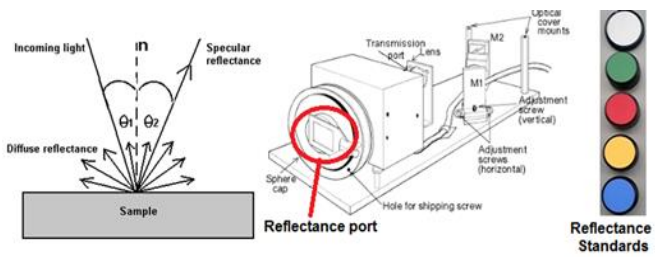
WHY USE UV/VIS SPECTROSCOPY?

- Provide quantitative information
- Rapid speed
- Non-invasive/non-destructive
- Little, to no, sample preparation

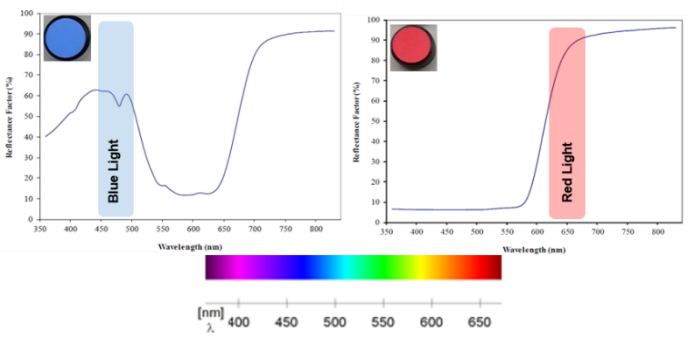
DIFFUSE REFLECTANCE ACCESSORY (DRA)

The DRA enables the user to characterise the reflectance of a solid material and determine the colour of the material.

A range of certified reflectance standards are available.



Reflectance spectra of blue and red standards as measured on a Cary 5000 using the DRA



WHAT IS IT?

A spectroscopic technique used to quantify the amount of specific analytes in a sample at a single wavelength.

A full spectral scan can also be obtained using this technique to identify multiple absorbance bands in a sample.

Results are usually generated in a spectral format with wavelength on the x-axis and either absorbance or reflectance on the y-axis.

Cary 5000©

SPECIFICATION / ATTACHMENTS

Agilent Cary 5000

- 175 -3300 nm wavelength range
- Up to 8.0 Absorbance units
- Variable slit widths down to 0.01 nm
- Sample holders for liquids and films
- Internal diffuse reflectance accessory (DRA) for reflectance measurement from solid samples
- Full WinUV software suite for: Colour, Concentration, Dissolution, Simple Scans and Full Spectral Scans

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.agilent.com

BRUKER AVANCE III 400 MHz NMR

SAMPLE TYPE

This NMR has a solution based probe. Thus all samples need to soluble in a deuterated solvent to an acceptable concentration.

The correct nuclei must be present in the sample in some abundance. The lower the abundance the higher concentration of sample is required.

The most common nuclei submitted for analysis are 1H and 13C. These are relatively common and so easily observable.

HOW NMR WORKS

The principle behind NMR is that many nuclei have spin and all nuclei are electrically charged. If an external magnetic field is applied, an energy transfer is possible between the base energy to a higher energy level (generally a single energy gap). The energy transfer takes place at a wavelength that corresponds to radio frequencies and when the spin returns to its base level, energy is emitted at the same frequency. The signal that matches this transfer is measured in many ways and processed in order to yield an NMR spectrum for the nucleus concerned.

The precise resonant frequency of the energy transition is dependent on the effective magnetic field at the nucleus. This field is affected by electron shielding which is in turn dependent on the chemical environment. As a result, information about the nucleus' chemical environment can be derived from its resonant frequency.

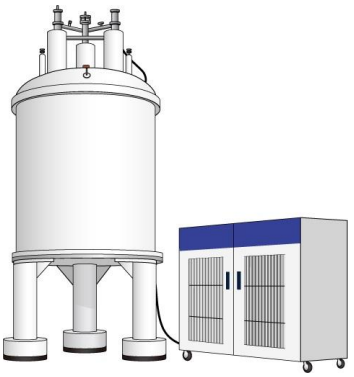
TASKS AND APPLICATIONS

- Analysis of purity
- Structure elucidation
- Molecular conformation in solution
- Studying physical properties at the molecular level such as conformational exchange, phase changes, solubility, and diffusion

WHAT IS IT?

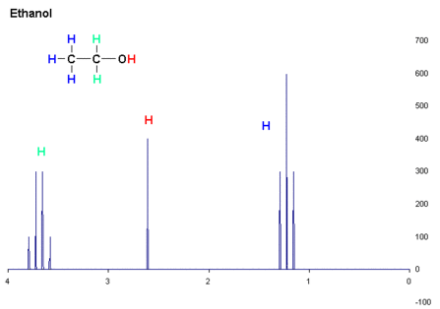
Nuclear Magnetic Resonance (NMR) spectroscopy is an analytical chemistry technique used in quality control and research for determining the content and purity of a sample as well as its molecular structure.

Once the basic structure is known, NMR can be used to determine molecular conformation in solution.



SPECIFICATION / ATTACHMENTS

- Temperature controlled probe
- Multinuclear probe
- Autosampler



QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.bruker.com

DIFFERENTIAL SCANNING CALORIMETRY

SAMPLE TYPE

The Discovery DSC can measure a range of different samples. The amount of sample required is determined by the property to be measured, but it is typically in the range of 1-10 mg.

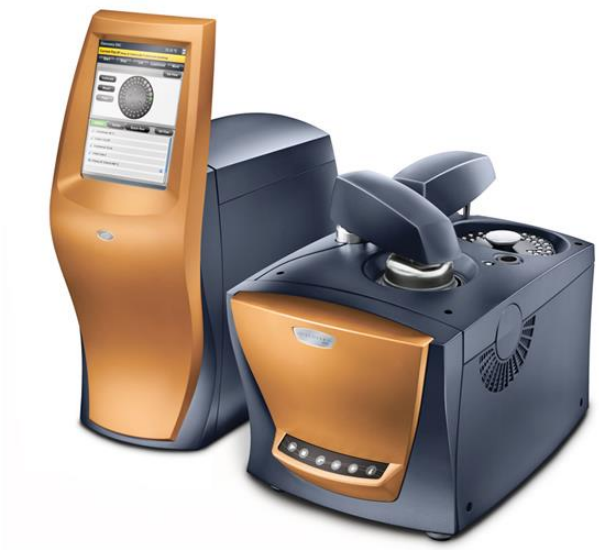
WHAT IS IT?

The TA Instruments Discovery Differential Scanning Calorimeter (DSC) measures temperatures and heat flows associated with thermal transitions in a material. Properties measured by TA Instruments' DSC techniques include phase changes, glass transitions, melting, crystallization, purity, heat capacity and oxidative stability. This information helps to identify processing and end-use performance.

Discovery DSC©

WHY USE THE TA INSTRUMENTS DISCOVERY DSC?

- Tzero® Press and Pans for fast, simple and reproducible sample preparation
- Discovery DSC AutoLid for more accurate and reproducible measurements
- Gas delivery module is capable of switching between two different purge gases at any point during an experiment
- User friendly interface with customizable view panels



Discovery DSC©

SPECIFICATION / ATTACHMENTS

- 54-Position Autosampler
- Temp. Range: -90 to 400°C
- Temp. Accuracy: ± 0.025°C
- Temp. Precision: ± 0.005°C
- Temp. Repeatability: ± 0.025°C
- Enthalpy Precision: ± 0.04%

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.tainstruments.com

KRUSS DSA100E DYNAMIC SHAPE ANALYSER

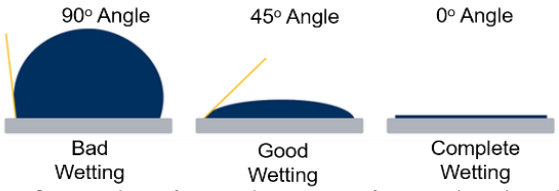
SAMPLE TYPE

The contact angle of millimetre and micrometre sized surfaces can be analysed using this system.

The surface tension of novel liquids can also be determined using the quadruple dosing unit.

WHY USE KRUSS DSA100E?

The water contact angle provides valuable information on the hydrophobicity of the sample.



The surface tension plays an important role in many different processes involving different phases and is particularly useful for emulsion stability and determining the tendency for phases to separate.

STANDARD VS MICRO CONFIGURATION

The standard configuration is suitable for both sessile drop and pendant drop measurements for the majority of samples.

Conversion from the standard into the micro configuration takes about one hour, however it allows far smaller dosing and the ability to measure the contact angle on smaller samples, for example hair fibres.

The micro configuration uses a Microdrop Technologies piezo system to dose 20 pL droplets and a more advanced x20 digital camera to capture the image before it evaporates (<1s).

WHAT IS IT?

The Kruss DSA100E is a fully automated software controlled instrument for the measurement of contact angles of solids using the sessile drop method and surface tensions using the pendant method.

The standard configuration can dispense 1-200 µL volumes onto millimetre sized samples whereas conversion to the micro system allows smaller doses of 20 pL to be dispensed onto samples in the micrometre range.

Kruss©

SPECIFICATION / ATTACHMENTS

Kruss DSA100E

- Software controlled x,y,z stage
- Software controlled dosing unit
- Camera with 1200 x 800 pixels at 200 fps
- Both surface contact angle and surface tension analysis
- Conversion to the micro system enables 20 pL dosing onto micrometre sized substrates

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.kruss.de

MICROMERITICS 3-FLEX

SAMPLE TYPE

This 3-Flex 3500 multi-port high throughput gas adsorption analyser is configured with two micropore and one mesopore port allowing the measurement of high resolution isotherms in the low pressure region.

A range of analysis gases can be used including:

N_2, O_2, Ar, Kr, Co_2, CO, H_2 and butane.

WHAT DOES THE 3-FLEX MEASURE?

Pore Size

Microporous materials have pores smaller than 2nm in diameter.

Mesoporous material contains pores with diameters between 2-50nm.

Macroporous materials have pores larger than 50nm in diameter.

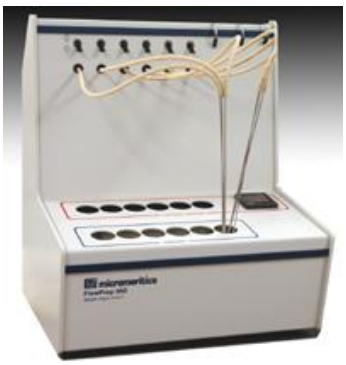
Chemisorption or Physisorption?

Chemisorption involves a chemical reaction between surface and adsorbate.

Physisorption involves very weak (van der Waals forces) forces between surface and adsorbate.

FLOWPREP 060 SYSTEM

The FlowPrep 060 is used to prepare your samples prior to analysis by applying both heat and a stream of insert gas to the sample. The heat desorbs any contaminants from the surface and the stream of insert gas sweeps them out of the tube. Specific temperature, gas and flow rate can be specified for optimal sample preparation.



Micromeritics©

WHAT IS IT?

A fully automated, three-station instrument designed for a variety of analysis including:

- Surface Area
- Mesopore
- Micropore
- Static and Dynamic Chemisorption
- Heat of Adsorption

Micromeritics©

SPECIFICATION / ATTACHMENTS

- Surface Area Range: 0.0005 m^2/g and above
- Pore Diameter Range: 3.5-5,000 Å
- Micropore Volume: Detectable within 0.001 cc/g
- The FlowPrep 060 system can degas up to 6 samples at temperatures up to 400°C using the flowing gas method

QUESTIONS? - CONTACT US.

mifinfo@liverpool.ac.uk

0151 795 7100

Supplier website: www.micromeritics.com