Q-Tof ™ 2

Q-Tof™ 2 is a new type of mass spectrometry tool for peptide sequencing, and protein characterisation and metabolite identification, a powerful alternative to the conventional triple stage quadrupole.
Q-Tof™ 2 is a high-sensitivity detector for on-line liquid chromatography - mass spectrometry (LC-MS and LC-MS-MS).
Q-Tof™ 2 is a compact, easy-to-use system featuring a straightforward user interface, incorporating a wealth of security, automation and biopolymer sequencing tools all running in Microsoft Windows NT®.

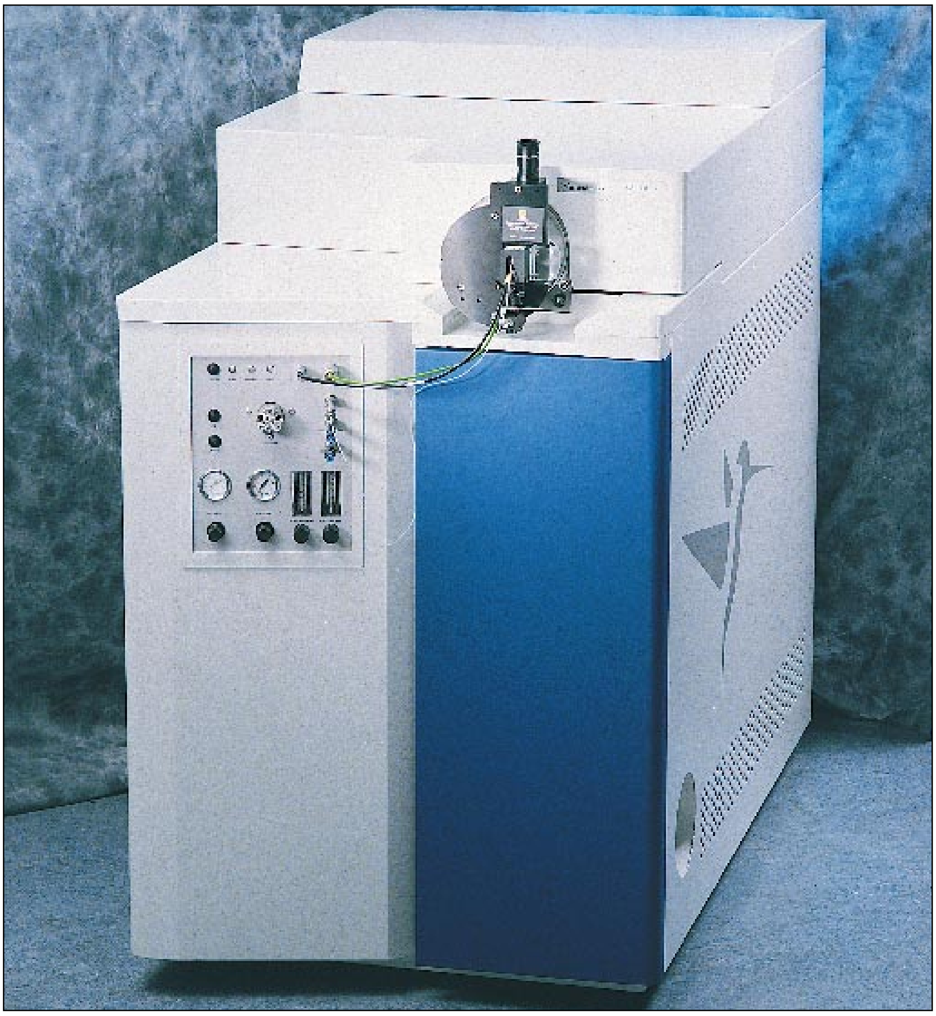
The orthogonal acceleration geometry exploited by Q-Tof™ 2 allows parallel detection of ions across the full mass range from a continuous ion beam. This is in contrast to conventional instruments that must scan over one mass at a time.

The net result ..... Q-Tof™ 2 delivers up to a 100 fold gain in sensitivity.

At the same time mass resolution in excess of 10 000 (FWHM) enables accurate mass measurements to be obtained in both MS and MS/MS modes.

Masslynx 3™ enables full integration of Q-Tof™ 2 with a wide range of solvent delivery and sample handling systems.

Masslynx 3™ is the benchmark for biochromatography-MS data handling. Each applications module in the MassLynx™ family has been written in collaboration with leading bioanalysts - ensuring a degree of intelligent integration previously absent in “Mass Spectrometry” data systems.



Protein identification is made easy with Micromass® optional BioLynx and ProteinLynx software packages.

Metabolite identification is made easy with Micromass“ optional Metabolynx software package.

Z Spray™

Z Spray™, Micromass’ quantum leap in robust API inlet technology is featured on Q-Tof™ 2 providing complete flexibility of analysis from small molecules to intact proteins with electrospray (ES), NanoFlow ES and atmospheric pressure chemical ionisation (APcI) options.

micromass®

Specification

Hardware

LC Interface

Atmospheric pressure ionisation source for sample introduction via Electrospray (ESI) and/or Atmospheric Pressure Chemical Ionisation (APcI) inlet probes allowing flow rates of 5-1000µL/min (ESI) and 200-2000µL/min (APcI). Samples may be introduced by direct infusion in solution, or the system may be interfaced directly to a HPLC system. The ion source incorporates a hexapole ion bridge to maximise transmission of ions from atmospheric pressure into the analyser.

Analyser

The first analyser consists of a precision engineered molybdenum quadrupole mass filter. A prefilter is fitted to prevent contamination of the main filter rods. An enclosed hexapole collision cell is included for high efficiency MS/MS fragmentation. The second analyser comprises a two stage orthogonal extraction region and linear reflectron for high resolution performance.

Detectors

Microchannel plate ion counting detector system for detecting positive and negative ions and acquiring both MS and MS/MS data.

Dynolite photomultiplier detector with conversion dynode and phosphor for optimising the ion source and first analyser transmission.

Vacuum System

Fully automated, differentially pumped vacuum system using 3 water cooled, 250 L/hr turbomolecular pumps for source, quadrupole and TOF housings. An isolation valve is situated after the sampling cone allowing rapid source cleaning without breaking vacuum.

A single E2M28 rotary backing pump is used.

Data System

Compaq Professional workstation AP200, 550MHz Pentium III, 128MB RAM, 9.1GB Wide-Ultra SCSI HDD, 32xCD ROM ELSA Gloria Synergy+Graphics.

MS Operating System

The system is controlled using the Micromass MassLynx NT™ operating system incorporating manual and automated instrument optimisation; automated instrument calibration; MS acquisition; MS/MS acquisition; selected ion monitoring via reconstructed mass chromatograms; chromatogram and spectrum processing. HPLC pump and autosampler control; photodiode array detector control and data acquisition;' '3D' data mapping; comprehensive quantitation package.

Security

MassLynx NT™ contains an advanced security system and features designed to aid GLP compliance including: password protected multi-level user accounts; logging of all LC-MS acquisition parameters; logging and time stamping of method modifications and data manipulation; secure audit trail.

Options

Open Access

OpenLynx LC provides a non-expert, walk-up system for the analysis of single compounds or simple mixtures for the automated determination of molecular weights and structural information. The system may be customised using factory produced software modules and includes a separate login PC to give maximum system security and ensure data integrity.

OpenLynx Diversity

Designed for the analysis of single compounds or simple mixtures produced by combinatorial chemistry or multiple parallel synthesis. Samples may be introduced from a variety of autosamplers, but the most usual method of sampling is from 96 well microtitre plates using a Gilson autosampler under Masslynx control. OpenLynx Diversity provides confirmation of the presence of expected molecular weights and produces reduced data sets and for simple data interpretation.

MetaboLynx (Automated Metabolite Identification)

MetaboLynx automatically processes data to search for expected and unexpected metabolites from an LC-MS acquisition using user-defined thresholds for peak intensity, spectrum purity and exact mass measurement. A control sample comparison may also be used to exclude matrix-related compounds. Moreover, it will set-up an MS/MS acquisition method containing the potential metabolite information ready for the subsequent acquisition of product ion spectra by LC-MS/MS. Optional DAD (Diode Array Detector) or analog inputs enable fully integrated data sets to be acquired and processed. The results are reported in a browser format that allows quick and efficient review of the data. The processing method is user configurable to allow the system to be applied to *in vitro* or *in vivo* studies.

ProteinLynx (Automated Protein Identification)

ProteinLynx automatically processes MS/MS data into a database query for the client-server ProteinProbe search engine. Results are returned in an interactive browser format that allows quick and efficient review of the results. Search parameters may be modified to refine the results or match previously unmatched data.
Data may be acquired using on-line chromatography and data dependent MS to MS/MS switching for fully automated protein identification. Protein Lynx incorporates the BioLynx tool kit.

BioLynx

A suite of software tools for the interpretation of data produced from the analysis of proteins, peptides and oligonucleotides including: amino acid sequence editor, nucleic acid sequence editor, EMBL CD-ROM library compatibility, protein mass fingerprinting, protein digestion simulators, hydropathic profiles.

ProteinProbe interactive client-server database search engine compatible with the SwissPROT protein database and any other FASTA formatted protein, oligonucleotide or EST database.

MassSeq (*de novo* peptide sequencing package)
MassSeq uses a rigorous probabilistic algorithm to deduce *de novo* peptide sequence from the ESI-MS/MS spectrum of peptides, typically derived from protein digests.

MaxEnt
Using Maximum Entropy processing applied to mass spectrometry data. MaxEnt aids the enhancement of complex spectra. MaxEnt 1 allows the deconvolution of overlapping multiply-charged spectra produced by the analysis of protein mixtures and glycosylated proteins. MaxEnt 2 Reconstruct gives enhanced resolution of m/z data within the mass range of the mass spectrometer to give unambiguous assignment of the charge state of multiply-charged peaks. MaxEnt 3 is used to deconvolute multiple charge state MS/MS data to a single charge state and subsume higher mass isotopes into the lowest mass isotope peak. The resulting data is used for *de novo* peptide sequencing or database searching.

Performance Specifications

Mass Range
Exceeding 20,000 Daltons.

Mass Resolution
10,000 (FWHM) on $(M+6H)^{6+}$ from bovine insulin.

Full scan MS sensitivity
Full scan MS sensitivity
(i) Positive ion mode
The signal height obtained from a sample consumption of 200 fmol of horse heart myoglobin (16952 Da) will be greater than 166 ion counts (equivalent to 600 ion counts at 1GHz sampling frequency) on the most intense peak in the charge state envelope. A solution of 200 fmol/mL horse heart myoglobin in 50/50 acetonitrile/water + 0.2% formic acid will be infused at a flow rate of 5mL/min.

(ii) Negative ion mode
The signal to noise obtained from the sample consumption of 1 ng of raffinose will be greater than 200:1. A solution of 5 ng/mL raffinose in 50/50 acetonitrile/water (no additives) will be introduced at 10mL/min. The signal to noise ratio will be measured on the $(M-H)^-$ peak at m/z 503.

Mass Measurement accuracy (with internal reference)
The mass measurement accuracy of the Q-Tof™ 2 under normal operating conditions, when at least one suitable peak of known mass is present and which can be used as an internal reference, is such that the RMS error between the measured and the accepted masses of peaks which have sufficient intensity and are free from interference from other masses will be less than 5 ppm over the range from 150 - 900 daltons.

Acquisition Rates
(i) oa-TOF pulse repetition rate
Variable up to 30,000 spectra/sec.

(ii) Histogrammed spectra acquisition rates over the range m/z 100 - 1000
a) Up to 4 spectra/sec for continuum (profile) spectra at 3.6GHz TDC rate.

Precursor ion selection mass range in MS/MS mode
Up to m/z 4000.

Precursor ion mass selection in MS/MS mode
Variable down to 1 dalton at m/z 1000.
Variable down to 2 dalton at m/z 2000.
Variable down to 3 dalton at m/z 3000.

Full scan sensitivity in MS/MS mode
The signal to noise from a consumption of 20 fmol of $[Glu^1]$ -Fibrinopeptide B (1569 Da) from a solution of 100 fmol/µL and at flow rate of 5µL/min will be greater than 30:1 on the most intense y″ sequence ion from the MS/MS spectrum of the doubly charged precursor ion.

Options

(A) Nanoflow electrospray
Full scan sensitivity in MS/MS mode

The signal to noise from a consumption of 2 fmol of $[Glu^1]$ -Fibrinopeptide B (1569 Da) from a solution of 500 fmol/µL concentration in MeOH/H_2O + 0.2% formic acid solution, using glass micropipettes with 1 or 2µm tips, will be greater than 30:1 on the most intense y″ sequence ion from the MS/MS spectrum of the doubly charged precursor ion. The integration period per spectrum will be about 5 sec and data will be summed over a period appropriate for the required consumption of sample.

(B) Transform software
(Software for the determination of molecular weight from a spectrum containing a series of multiply charged ions on an m/z scale by a transform of the data to a true mass scale.)

Mass measurement accuracy (no internal reference)
Measured from the mean of five repeat analyses of the globin from normal human haemoglobin. Mass calibration to be performed using the multiply charged globin peaks from a separate analysis. The mean measured mass shall be 15867.2 +0.5 Da and the standard deviation of the mean <0.5 Da. It is recommended that a solution containing

Installation Requirements

Power requirements

The instrument requires a single phase 50 - 60 Hz, 230V nominal power supply rated at 13A (UK) or 15A (Europe).

In the USA and Canada a single-phase 50 – 60 Hz supply at 230V phase to neutral fused and rated at 15A is required. Alternatively two phases of a 50 – 60 Hz 208V phase to phase, 3 phase supply, rated and fused at 15A may be used.

An optional transformer is available to accommodate other supply voltages.

Power consumption

Typical power consumption excluding ancillary equipment (computer, LC etc.) 1.5kW.

Water supplies

The heat dissipated into the cooling water is about 400 Watts. The typical water flow required to dissipate the heat generated by the turbo pumps is 35 L/hour for an inlet temperature of about 20 ^{0}C or 23 L/hour at an inlet temperature of about 15 ^{0}C assuming an outlet temperature of about 30 ^{0}C.

Gases and regulators.

Nitrogen:

Dry nitrogen, oil free supply regulated at 7 bar (100 psi) minimum outlet pressure to provide
nebulising and drying gas to the instrument

Collision gases:

Typically argon is used as the collision gas for CID experiments other gases may be used if required.
Supply must be pressure regulated at 50psi max.

Environment

It is recommended that the instrument is sited in an air conditioned laboratory, in a draught free position and away from excessive amounts of dust.

The maximum ambient laboratory temperature should not exceed 30 ^{0}C (86 ^{0}F), optimum temperature lies in the range
19 - 22 ^{0}C (66 -72 ^{0}F). Short term (1.5 hour) variations should be no more than 2 ^{0}C.

The relative humidity should not exceed 70%.

Heat dissipated into the laboratory from the instrument is about 1.2 kW.

The instrument conforms to IEC 1010 - 1 Pollution Degree 1 and Installation Category II.

Exhausts

Separate vents are required to remove the API gas exhaust and rotary pump exhaust from the laboratory.

Room size and access requirements

The Q-Tof™ 2 analyser unit is 730 mm (28.5 inch) wide by 1320 mm (52 inch) deep and weighs 500 kg (1100 lb). It is mounted on 4 rolling casters, which allow the instrument to be easily transported over smooth surfaces.

A separate table 1200 mm (47 inch) by 730 mm (28.5 inch) is supplied for the computer terminal.

Doorways through which the instrument is to be transported should be a minimum of 770 mm (30.5 inch) wide.

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The Mass Spectrometry People

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