The finest Q-Tof™
Introducing the ultimate
technology for
tandem mass spectrometer
API LC-MS-MS
for research in the USA

www.micromass.co.uk
Maximising Data Quality and Knowledge

Mass-Informatics™ enables chemically meaningful knowledge to be extracted “in silico” from multi dimensional datasets (e.g. m/z, intensity, retention time) automatically. Micromass’ latest Mass-Informatics™ system (MassLynx™ 4.0) circumvents “raw data mountain syndrome” in high throughput ADME, drug impurity or proteomics studies. However, the power of Mass-Informatics™ to automatically deliver authenticated answers is constrained by raw data quality - “excellence in ... excellence out”.

The quest for knowledge rather than “just” data in high throughput post-genomic studies is forcing a new analytical paradigm in visionary scientific enterprises.

API MS-MS instruments with traditional “data systems” that efficiently converted sample mountains into raw data mountains are being superseded with networked “Sample to Knowledge” converters like Micromass’ new Q-Tof™ API-US. These new systems are a fusion of “intelligent” high performance mass analysers and client-server Mass-Informatics™ leveraged with the largest portfolio of compatible software platforms...from the Global e-MS™ Consortium.

Introducing the superpremium LC-MS-MS for...
Micromass’ classic Q-Tof™ defined this instrument category in 1996 - delivering unprecedented sensitivity, selectivity and speed of analysis in LC-MS-MS. Today’s Q-Tof™ API-US takes the sensitivity, resolution and mass measurement accuracy of Micromass’ classic Q-Tof™ concept to new heights... delivering the most excellent LC-MS-MS data available to maximise Mass-Informatics™ productivity.

Key features of the Q-Tof™ API-US:
- **Z SPRAY™** ...the world’s leading high performance ion source for rugged APCI & ESI
- **WOPTICS™** for high resolution - 17,500 FWHM
- **Data Directed Analysis (DDA™)** for dynamic Precursor Ion Discovery
- **Dynamic eXternal Calibration (DXC™)** for exact mass measurement in fluctuating thermal environments
- **LockSpray™** enabled 5ppm exact mass measurements
- **Digital DeadTime Correction (DDTC™)** technology for quantitation ~10⁴
- **Integrated syringe pump with full digital control**
- **Digital flow control of source gases**
- **Electronically controlled sample injection valve**
- **MassLynx™ 4.0** ...the market leading Targeted Mass-Informatics™ platform
- **Access to the most popular 3rd party software from the Global e-MS™ Consortium**

Micromass’ Q-Tof™ API-US is the exact mass LC-MS-MS system of choice for metabolism studies, proteomics and structural analyses in the post-genomic era.
The Q-Tof™ API-US is the ultimate expression of Micromass’ Quadrupole / orthogonal acceleration Time-Of-Flight (Q/oa-TOF) concept - enhanced with WOPTICS™ technology.

The Q-Tof™ API-US combines the simplicity of a quadrupole [MS 1], the high ion conductance of a hexapole collision cell and the ultra high efficiency of an oa-TOF mass analyser [MS 2]. Q-Tof™ API-US exploits oa-TOF MS to achieve simultaneous detection of ions across the full mass range. This is in contrast to conventional instruments that must scan over one mass at a time. Q-Tof™ API-US offers up to 100 times more sensitivity than tandem quadrupole instruments when acquiring full product ion (MS-MS) mass spectra - essential for confident assignment in metabolism studies and peptide characterisation.

The oa-TOF mass analyser has an upper m/z range of 20,000 and a resolution of 10,000 FWHM in both MS and MS-MS modes - increased to 17,500 with Micromass’ exclusive WOPTICS™ option.

The Q-Tof™ API-US delivers solutions for optimum sensitivity and resolution. The programmable TOF analyser geometry under MassLynx™ control allows a simple switch from ‘VOPTICS™’ to ‘WOPTICS™’ mode - delivering increased resolution with the click of a mouse. The activation of an additional ion mirror within the analyser enables an extended flight path to be achieved with an additional pass through the main reflectron. This increases the effective path length of the instrument, while maintaining spatial focus - delivering enhanced resolution at maximum sensitivity.

Q-Tof™ API-US delivers automatic exact mass measurement over a wide, quantitative dynamic range (\(\sim 10^4\)) at full sensitivity - enabled by Digital Dead Time Correction (DDTC™) technology in conjunction with a continuous, large surface area MCP detector.
“... for materials with molecular weights below 1000, the measured mass should generally agree to 5ppm or better, with the calculated mass.”

Notice to Authors of Papers:  J. Am. Chem. Soc., 1999, 121(1), 7A-12A

\textbf{ZSPRAY™}

Q-Tof™ API-US features Micromass’ patented \textbf{ZSPRAY™} Atmospheric Pressure Ionisation (API) inlet technology for LC-MS-MS. The dual orthogonal geometry of \textbf{ZSPRAY™} enables prolonged LC-MS-MS analysis of samples in complex biological or environmental matrices. The interface supports both MegaFlow™ and NanoFlow™ inlet options.

Over 3500 \textbf{ZSPRAY™} based instruments have been installed in laboratories worldwide, making it the number one high performance API LC-MS interface.

\textbf{Exact Mass LC-MS-MS}

The masses of small ions (< m/z 1000) in both MS and MS-MS spectra can be measured routinely to within 5ppm RMS, in the presence of a known lock mass. Q-Tof™ API-US features Micromass’ LockSpray™ / NanoLockSpray™ dual ESI interface options for the optimised co-introduction of analytes and a lock mass compound to deliver authenticated exact mass measurements spectrum by spectrum in both MS and MS-MS modes.

In the absence of an internal reference, mass measurements can be achieved to within 10ppm RMS with Micromass’ Dynamic eXternal Calibration (DXC™) technology - counteracting variations in laboratory temperature.
Q-Tof™ API-US runs MassLynx™ 4.0 - the latest version of the market leading mass spectrometry software from Micromass-Waters, the pioneers of Mass-Informatics™. MassLynx™ 4.0 is optimised for Microsoft Windows XP and functionally validated for Windows NT / 2000.

With over 1000 refinements, MassLynx™ 4.0 introduces the ‘targeted’ Mass-Informatics™ concept. Featuring a ground breaking context sensitive user interface, MassLynx™ 4.0 makes the most powerful mass spectrometry techniques accessible - with Application-Managers™ optimised using simple 'customisation wizards'.

**Application-Managers™**

The ‘core Mass-Informatics™ engine’ of MassLynx™ 4.0 can be enhanced with a range of optional ‘plug-in’ Application-Managers™ for many key tasks in pharmaceutical and life science research (e.g. proteomics and metabolism studies).

The Application-Managers™ enable each user to effortlessly select and augment only the relevant tools from the powerful ‘core Mass-Informatics™ engine’ - enabling the analysts to focus the full power of targeted Mass-Informatics™ on their challenge with the minimum training overhead.

**Leveraging with Exact Mass**

Q-Tof™ API-US leverages the power of Mass-Informatics™ with exact mass data enabling the elemental compositions of molecular or fragment ions (MS-MS) to be confirmed for postulated compounds - allowing nominally isobaric species to be differentiated. For “unknowns” the number of plausible elemental compositions may be restricted to a small number, or uniquely identified, with the aid of additional chemical/biological information (e.g. known synthetic route or viable in vivo bio-transformations).

The Global e-MS™ workspace

Many scientific enterprises are adopting common platforms to facilitate virtual integration of knowledge from a multiplicity of sources. Windows NT, HTML and XML...
are enabling this process - providing the *de facto* standard for the Global e-MS™ Consortium’s workspace. MassLynx™ 4.0, Micromass’ groundbreaking targeted Mass-Informatics™ technology, provides the exclusive MS vendor portal to the Global e-MS™ workspace ...with the largest portfolio of compatible software platforms.

...the exact standard in targeted Mass-Informatics™
The Data Directed Analysis (DDA™) / Precursor Ion Discovery modes of the Q-Tof™ API-US make it ideally suited to identification of a wide range of compounds. From full scan LC-MS searching for unknown components, to class-specific identification based on precursor ion discovery by neutral loss, through to exact mass, full product ion MS-MS to confirm structural elucidation.

Micromass' MetaboLynx™ Application-Manager™ features advanced tools to extract meaningful information from these complex data sets, distilling large LC-MS raw data files into simple, manageable reports. Using innovative control sample comparison and combined chromatographic and spectral searching, MetaboLynx™ easily identifies new components, flagging them as potential metabolites or impurities.

Further investigation can be carried out by automatically scheduling MS-MS analyses on flagged components. Data Directed Analysis™ may also be employed to acquire LC-MS and MS-MS information from a single experiment and processed by MetaboLynx™ to reveal structural similarities between metabolites and their parent drug.
Data Directed Analysis

In on-line LC-DDA-MS analyses the Q-Tof™ API-US continuously records “MS survey” spectra throughout a chromatographic run to dynamically discover candidates for full product ion analysis (MS-MS). When a component of interest elutes the m/z value of the molecular ion is first determined, the quadrupole mass analyser then switches to transmit the “discovered” precursor ion (m/z) only for MS-MS analysis. After the MS-MS analysis is complete the system returns to the MS survey to hunt for the next component of interest.

Automated Precursor Ion Discovery requires the definition of one or more criteria for selection and/or rejection of candidate precursor ions. These criteria may include:

- selection based on required charge state
- selection based on relative or absolute intensity
- selection based on list of preferred / excluded m/z values, either nominal or exact
- rejection based on temporary (dynamic) list of excluded m/z values

When ‘MS survey’ spectra are acquired sequentially at alternate high / low (CID) collision energy two additional selection criteria for precursor ion discovery in real-time are enabled:

- selection based on the presence in the high collision energy ‘MS survey’ spectrum of a specific product ion m/z value (nominal or exact).
- selection based on the detection (within sequential low/high energy ‘MS survey’ spectra) of pairs of ions with a specific nominal or exact difference in m/z (neutral loss).
Micromass’ ProteinLynx™ Global SERVER 2.0 defines a new software category ‘the total protein Mass-Informatics™ platform’, featuring a new and comprehensive range of integrated tools for proteomics project management, protein quantification and protein identification, leveraged with the specificity of exact mass data ...more than ‘just’ a search engine!

ProteinLynx™ is optimised for use with Micromass’ M@LDI™ and Q-Tof™ families of high performance mass analysers in multi-instrument laboratories. The System offers an automated hierarchical approach to protein identification for fully unattended data interpretation. In addition, ProteinLynx™ can support ‘walk up’ protein analyses in multi-user/multi-laboratory research environments.

The project management tools provided with ProteinLynx™ allow thousands of samples to be catalogued, annotated and tracked from their biological origin through to their identification and quantification by mass spectrometry. In a further advance, protein spots in imported 2D gel images may be annotated with assigned protein IDs and co-presented with the supporting MS evidence.
ProteinLynx™ takes full advantage of exactly mass measured, high resolution MS-MS data to maximise selectivity when interrogating databanks of known proteins, in the automatic detection of PTMs and in de novo sequencing. Protein/peptide identification strategies can be chained together in an automated, hierarchical WorkFlow™. Peptide/protein spectra that cannot be matched to the databanks with high probability are automatically de novo sequenced and submitted for homology analysis with ProteinLynx’s on-board BLAST® search engine.

Remotely accessible results through an intuitive web browser enable each user to securely log-on to their own (password protected) projects. Confidentiality is assured with an encrypted file format. The browser allows results to be reviewed and additional databank interrogations to be initiated remotely with modified search parameters.

ProteinLynx™ features a scalable 3-tiered client-server architecture and is compatible with AIX (IBM), Solaris (Sun), Linux and Windows® XP, NT & 2000 operating systems and the industry standard Oracle and DB2 relational database systems.

For the first time, ProteinLynx™ Global SERVER 2.0 provides an integrated platform to manage multi-technique analytical strategies, automatically interpret the resulting MS data and make complex data sets accessible to proteomics researchers...

...the total protein Mass-Informatics™ platform!
As a Q-Tof™ API-US user you’ll have the reassurance of our professional training programs and global service network. Service contracts can be customised to meet individual needs and can include guaranteed response time, preventative maintenance schedules, MassLynx™ upgrades and telephone support. Supplement this with Micromass’ new on-line resources including manuals, parts, software, instrument and applications literature. Micromass’ commitment to customer satisfaction is complete and unequivocal.