



QTOF MS

Unique features of the Drug Screen Suite



PROPERTIES

Mass Spec

- The MS instrument is a benchtop, small footprint, easy-to-use high-resolution electrospray ionization quadrupole time-of-flight GC (optional) and LC mass spectrometer designed for exact mass and true isotopic measurements at a speed enabling data acquisition on chromatography-free DART shots or at UHPLC speed for both MS and MS/MS mode.
- The Vacuum Insulated Probe (VIP) dual source including VIP Heated Electrospray (HESI) and Atmospheric Pressure Chemical Ionization (APCI) probes for unreached sensitivity for many compounds of interest in the fields of environmental analysis, food testing and forensic drug investigations and proven robustness in routine analysis in 24/7 operation.
Flow rate: 3 – 2,000 $\mu\text{L}/\text{min}$.
The probe sprayer design separates the heated gases from the eluent stream by a thin evacuated space, saving thermo-labile compounds from degradation.
- Active Exhaust technology of the VIP-HESI ion source is preventing spray or vapor to re-circulate in the ion source. This results in lesser chemical background noise and reduces the need for source cleaning.
- Close to orthogonal ESI sprayer needle for reduced noise allowing flow rates from 1 – 1,000 $\mu\text{L}/\text{min}$. ESI source needle must be at ground potential for easy coupling with UHPLC and capillary electrophoresis.
- Patented dual ion funnel for maximum ion transmission and instrument sensitivity in the first pump stages and for a wide m/z transmission.
- High performance hyperbolic quadrupole and broad mass transfer collision cell with full quadrupolar ion transmission up to m/z 40,000 (rf-only mode) and ion selection prior to MS/MS up to m/z 3,000. Both enable a broad range of applications from small molecules to polymers or proteins.
- In-flight refocusing optics, dual stage ion reflectron and high-sensitivity and fast ion detector system resulting in high performance analyzer resolution in single-reflection mode better than 30,000 (FWHM) at m/z 1,222 with a single stage V-reflection, without any loss of sensitivity (full sensitivity resolution) and independent of spectra acquisition speed.
- MS and MS/MS mass accuracy better than 0.8 ppm (calibrated internally) and 2 ppm (calibrated externally) in a wide dynamic range, i.e. independent from sample concentration.

- Only one calibration required for MS and MS/MS. The calibration is independent of the charge state of the calibrant. This is essential for confident identification or verification of compounds, by both determination of the elemental composition of comparison with libraries.
- Digitizer with 5 Gsample/sec Analog to Digital Converter (ADC) with 50 Gbit/sec and 10 bit dynamic range leading to an intra-spectral dynamic range of ≥ 5 orders of magnitude at 1 Hz data acquisition speed without any need to split the ion beam dynamically and without any need to switch the digitizer into under sampling mode.
- Possibility to create high resolution extracted ion chromatograms within ± 1.0 mDa error for screening of complex mixtures. This is essential for high selective measurements of targeted compounds, and to filter them from any kind of matrix background.
- Long-term robustness and a constantly high quality of the data suitable for 24/7 operation over several weeks, without the need to tune the detector in order to counterbalance contamination or aging. No time effects on peak areas, mass accuracies and isotopic pattern quality of compounds.
- Ability to determine target compounds at trace level using optional VIP-HESI ion source: sensitivity for reserpine 50 fg S/N > 150:1
- Scintillator-free Multi Channel Plate detector (MCP) for extremely long lifetime with neglectable aging effects.
- bbCID for all ion fragmentation with an alternating mode between MS and MS/MS.
- The MS instrument with (H)ESI source allowing positive and negative ion detection with the needle of the ESI source grounded for safer operation.
- The MS instrument and accessories are integrated in otofControl/HyStar creating a complete package and ease of use concept. All analytical flow workflows like data acquisition in otofControl and control of Elute Plus LC systems and Bruker GC-system in HyStar. In case of CTC based autosampler a separate plug-in is fully supported.

Liquid Chromatography

- Robust state of the art pump with linear drive technology for two pairs of serially coupled pump heads for UHPLC chromatography precise solvent delivery, allowing
 - pressures up to 1,300 bar for flow rates from 0.001 to 2 mL/min
 - Flow gradient for optimum separation with flow accuracy: ± 1 % or ± 10 μ L, whatever is greater
 - High quality database with narrow RT windows driven by flow precision ≤ 0.075 % RSD or 0.005 min SD, whatever is greater
 - Integrated degasser and truly automated priming and purging for a reliable UHPLC pump and easy maintenance.
 - Equipped with active piston backflush to extend the lifetime of the seals and the pump. The degasser is integrated to the pump as well as an automated soft flow rate ramping option to guarantee best (U)HPLC column lifetime.
 - Autosampler with cooling and heating
 - Loop injection with injection range from 0 to 100 μ L in 1 μ L increments using 100 μ L standard loop (optional loops with following volumes can be used: 2, 5, 10, 50 μ L)

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- Carry Over: $\leq 0.001\%$ (Chlorhexidine) programmable wash procedure, to deal with various matrices and sample types.
- Injection needle wash: 2 solvents available, optional stator wash, inside and outside needle wash with drying. Wash can be programmed between injections and between vials/wells.
- Cycle time (injection to injection) < 20 sec.
- Temperature range 4-40 °C with temperature precision of ± 2 °C at 4 °C.
- Intermediate loop decompression technology valve results in maximizing column lifetime and avoiding unwanted sample dilution and pressure shocks through ultra-fast valve switching.
- Pressure assisted sample aspiration concept avoids sample-syringe contact and air bubbles.
- Sample Capacity 2 x 96 and/or 384 microtiter plates or 108 x 2 mL vials or 30 x 10 mL vials
- Column oven with cooling
- Temperature range: ambient -15 °C to 90 °C in 1 °C increments
- Optional column switching valve to best use column capacity of 6 columns; each up to 300 mm
- MarvelXACT™ fittings for reliable handling.

Software, Database and Methods

- The identification system allows highest speed by using ultra high performance liquid chromatography (UHPLC) coupled online with high resolution QTOF technology: the complete analysis time for one sample from injection into the LC-MS system, library search, data analysis and reporting is achieved below 20 min.
- Toxicology identification system based on a spectral library of drugs, drugs of abuse and metabolites with at least 340 most common toxic substances.
- The system must combine retention time (RT), high-resolution MS, and MS/MS information for the library search by an advanced algorithm for highest identification and confirmation at the same time.
- The external MMHW library must be fully supported by the library search algorithms taking MS, and MS/MS into account.
- Open library concept: the library must be extendable by the user and the insertion of new analytes and spectra must be fast and easy.
- The combined information of retention time and molecular mass must be considered in the acquisition software by a “scheduled precursor list” leading to an increased sensitivity compared to a “data dependent” acquisition approach.
- The sample management of the system until final report generation must readily be handled by non-LC-MS experts
- At the end of an analysis, reports must be given automatically via the software
- The data system holds User Action Rights to give certain access rights to the user (and admin). The system has no limitation in the number of licenses.
- Software needs to be based on client-server architecture including full floating client licenses .
- Intuitive, simplified user interface, easy to learn and master for users in routine testing.

SPECIFICATIONS

- Please see Spec Sheets.

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FUNCTIONS

Software Control

- Plugin for Elute plus UHPLC fully integrated in HyStar.
- Multi-dimensional data processing in retention time, intensity, and m/z .
- Automated in-batch recalibration in m/z .
- Fully automated isotope pattern matching with the generation of a list of the sum formula from both mass accuracy as well as the isotope pattern matching.
- Extracted Ion Chromatograms within +/- 1 mDa error for screening of complex mixtures

Ion Sources and Probes

- VIP-HESI source, ESI flow rate of 3 $\mu\text{L}/\text{min}$ – 2000 $\mu\text{L}/\text{min}$

PATENTS COVERING UNIQUE FEATURES

1. Electro-Spray Ion Source with Ion Funnel:

- **Title: “Ion guide for mass spectrometers”**
 - Issued: CA2463433C; CA2747956C; US7495212B2; US7851752B2; US8222597B2;
 - EP1465234B1 (DE, GB)
- **Title: “Ion funnel with improved ion screening”**
 - Issued: GB2402261B; US7064321B2

2. Ion Guide System

- **High Precision Multipole Rod Ion Guides**
 - Title: “Multiple rod systems produced by wire erosion”
 - Issued: DE102004037511B4; GB2416915B; US7351963B2

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- **Ion Beam Conditioning**

- Title: "Conditioning of an ion beam for injection into a time-of-flight mass spectrometer"
- Issued: GB2361803B; US6700117B2

3. TOF Mass Analyzer:

- **Gridless Orthogonal Accelerator and Ion Optics for Focus Mode**

- Title: "Gridless time-of-flight mass spectrometer for orthogonal ion injection"
- Issued: DE10005698B4; GB2361353B; US6717132B2

- **Ion Pulser**

- Title: "Pulsers for time-of-flight mass spectrometers with orthogonal ion injection"
- Issued: DE10158924B4; GB2386751B; US6903332B2

- **Reflector Design**

- Title: "Reflectors for time-of-flight mass spectrometers"
- Issued: DE102014009900B4; CN105244242B; US10026601B2; GB2530840B

- **Auto-Calibration of Detector**

- Title: "Method of adjusting the detector amplification in mass spectrometers"
- Issued: DE102008010118B4; GB2457559B; US8536519B2

- **Advanced Mass Band-Width**

- Title: "Method of operating a time-of-flight mass spectrometer with orthogonal ion pulsing"
- Issued: DE102011100525B4; GB2490577B; US8927928B2

4. Signal Processing

- **Threshold Filtering – Noise Reduction**

- Title: "Method and apparatus for producing mass spectrometer spectra with reduced electronic noise"
- Issued: DE10152821B4; GB2385982B; US6836742B2

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- **SNAP**
 - Title: “Mass spectrometry method for accurate mass determination of unknown ions”
 - Issued: DE19803309C1; GB2333893B; US6188064B1
- **Focus – High Mass Resolution Mode**
 - Title: “High resolution detection for time-of-flight mass”
 - Issued: DE10206173B4; GB2390936B; US6870156B2
- **Enhanced Quadratic Calibration**
 - Title: “Calibration curves for time-of-flight mass spectrometers”
 - Issued: DE102007027143B3; GB2454282B; US7851746B2

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