



QTOF MS

Unique features of the Seized Drug Suite



The Seized Drug Suite is a predefined combination of items. Amongst others this is a compact MS-system and a DART JumpShot ion source. The properties and features described as follows represent benefits to express preference for the offered product. Some features are optional.

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 Analog to Digital Converter (ADC) with 50 Gbit/sec and high 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.
- 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 enables reliable review of data
- 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 DART, Elute Plus LC systems and Bruker GC-system in HyStar. In case of CTC based autosampler a separate plug-in is fully supported.

Chromatography free DART ion source

- Robust 1- or 2-axis set up with motor driven sample holders for precise and fast movement
- Fixed 45° angle mount to enable off-axis experiment modules
- QuickStrip module for analysis of up to 12 samples using the QuickStrip wire mesh consumable with fixed positions automatically sampled precisely
- TLC plate module for prep and analytical plates
- Twelve position DIP-it module with microtiter plate spacing for high throughput sampling
- Multi Tablet Carrier package, holding up to 10 tablets for analysis

Bruker Switzerland AG
Fallanden • Switzerland
Phone +41 44 825 91 11

Bruker Scientific LLC
Billerica, MA • USA
Phone +1 (978) 663-3660

Online information
bruker.com

ms.sales.bdal@bruker.com



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- Tweezer module package enables precise method-based sampling of single tablets and other objects
- 3D Scanner sample stage with digital X-Y movement control and manual Z-direction setting. Can be mounted horizontally or vertically, to accommodate any sample
- Infusion module for sustained delivery of liquid analytes or dopants to ionization region
- Grid Voltage between 0 and 530 Volts for optimal transfer efficiency from source to mass spec
- Grid Voltage available in both polarities for widest possible applicability
- Temperature range: 0 °C to 500 °C in 1 °C increments covering techniques from volatile analysis to thermal desorption

Software, Database and Methods

- The identification system allows highest speed DART JumpShot sampling with high resolution QTOF technology.
- Identification system for controlled substances based on a spectral library of drugs and drugs of abuse with at least 270 most common drugs and drugs of abuse.
- The system must combine high-resolution MS, and MS/MS information for the library search 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 sample management of the system until final report generation must readily be handled by non-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.

FUNCTIONS

Software Control

- Plugin for DART fully integrated in HyStar.
- Multi-dimensional data processing taking
- Automated in-batch recalibration in m/z .

Bruker Switzerland AG
Fallanden • Switzerland
Phone +41 44 825 91 11

ms.sales.bdal@bruker.com

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Phone +1 (978) 663-3660

Online information
bruker.com



Ion Source

- DART Ion Source

PATENTS COVERING UNIQUE FEATURES

1. Ion Guide System

- **High Precision Multipole Rod Ion Guides**
 - Title: "Multiple rod systems produced by wire erosion"
 - Issued: DE102004037511B4; GB2416915B; US7351963B2
- **Ion Beam Conditioning**
 - Title: "Conditioning of an ion beam for injection into a time-of-flight mass spectrometer"
 - Issued: GB2361803B; US6700117B2

2. 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

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- **Advanced Mass Band-Width**

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

3. Signal Processing

- **Threshold Filtering – Noise Reduction**

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

- **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

4. DART ion source enabling chromatography free workflows

- **Ionization Principle**

- Title: "Method for atmospheric analyte ionization"
- Issued: US7112785 B2 – expired, fulfilled by DART ion source

- **General Hardware Setup**

- Title: "Atmospheric Pressure Ion Source"
- Issued: US6949741 B2 – expired, fulfilled by DART ion source

- **Efficient Ion Transfer – Improvement of S/N**

- Title: "Sampling system for use with surface ionization"
- Issued: US2007205362 AA

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- **Measures for improved surface sampling**
 - Title: “High resolution sampling system for use with surface ionization technology”
 - Issued: US2008067348 AA
- **Electrostatic ion guides for enhanced transfer**
 - Title: “Sampling system for containment and transfer of ions into spectroscopy system”
 - Issued: US2008087812 AA
- **Thermal desorption of Analytes**
 - Title: “Apparatus and method for thermal assisted desorption ionization systems”
 - Issued: US2012199735 AA
- **Sample positioning**
 - Title: “Robust, rapid, secure, sample manipulation before, during and after ionization for a spectroscopy system”
 - Issued: US8901488 BA
- **Chemical Fingerprinting**
 - Title: “Apparatus and method for generating chemical signatures using differential desorption”
 - Issued: US2015364310 AA
- **Sampling of different phases**
 - Title: “Apparatus and method for chemical phase sampling analysis”
 - Issued: US2019013190 AA
- **Independence from matrix effects**
 - Title: “Apparatus and method for reduction of matrix effects”
 - Issued: US2019371592 AA
- **Gas saving by JumpShot**
 - Title: “Pulsatile flow atmospheric real time ionization”
 - Issued: US2022013347 AA

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