KNAUER

One instrument for all applications

MSQ Plus™ – mass spectrometer for HPLC/UHPLC analysis

Robust solution

Rugged, easy to use, high-performance

Nowadays instrumental analysis in quality control and in research & development means unsupervised sample management as well as fast and reliable results.

Using the space-saving, fast and powerful MSQ Plus™ single quadrupole detector together with the high-performance PLATINblue UHPLC system, maximum productivity without compromises in terms of data quality, sensitivity and sturdiness can be achieved.

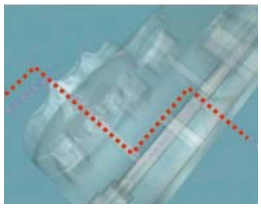
The Xcalibur™ software easily and comprehensively controls all LC and MS operating parameters, checks data and compiles result reports. As a matter of course, the software complies with 21 CFR Part 11.

Resolve routine tasks in a more efficient way

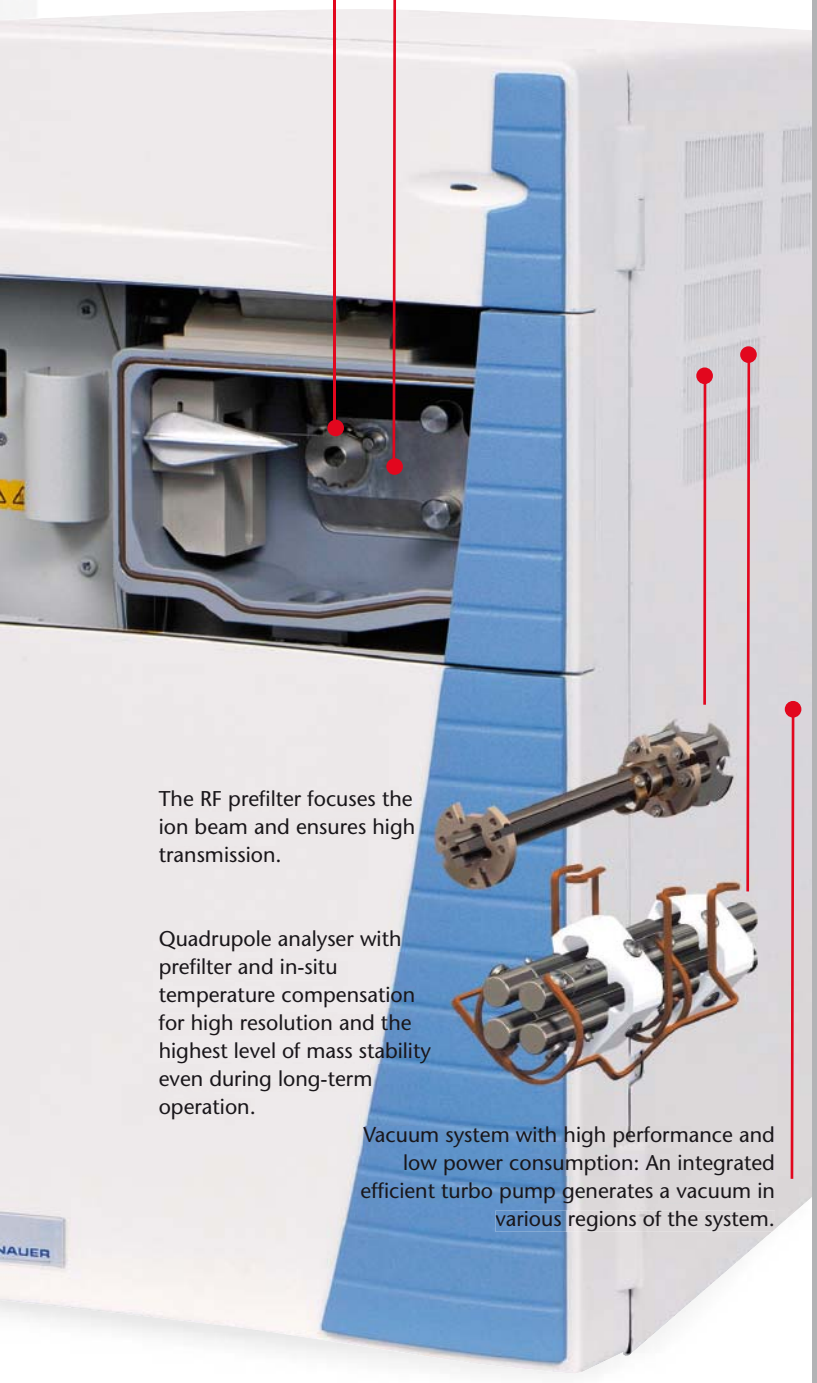
The MSQ Plus mass detector handles tasks that often require a lot of time in daily practice much easier due to fast and unique mass identification. With this device, quantitative analysis is more reliable and up to 1000 times more sensitive than UV detection. This means in everyday laboratory life:

- Improvement of the limit of detection and limit of quantification due to increased sensitivity and enhancement of the calibration range in contrast to conventional detection procedures..
- Faster method development compared with UV detection as unique results are generated.
- More reliable peak identification even from trace impurities or co-eluting peaks.
- Fast multi-component analysis and confirmation of molecular weights even when HPLC separation is insufficient.
- Simultaneous analysis of anions and cations possible in one run.

Automatic cleaning of sample inlet.



The triple „orthogonal“ M-Path™ design reduces neutral background for high sensitivity.



The RF prefilter focuses the ion beam and ensures high transmission.

Quadrupole analyser with prefilter and in-situ temperature compensation for high resolution and the highest level of mass stability even during long-term operation.

Vacuum system with high performance and low power consumption: An integrated efficient turbo pump generates a vacuum in various regions of the system.

Why I use the MSQ?

This MS detector interacts optimally with the PLATINblue HPLC/UHPLC system and facilitates considerably more determinations than systems with classic detectors. The system can be used for micro LC, HPLC and UHPLC. This MS detector supports flow rates of up to 2 ml/min without splitting.

The fast change in polarity function facilitates the determination of anions and cations in one run.

The ability to combine the scan and determination of individual ions facilitates identification and quantification in one run.

I can also obtain structural data as a result of the switchable collision-induced dissociation (CID) in the ion source.

The sample inlet is made of titanium making the MSQ Plus extremely robust and resistant to chemicals.

Automatic cleaning of the sample inlet reduces maintenance work and thus downtimes.

I am impressed with the simple operation and high performance. No tools or cables are needed to change the FastLoc ion sources.

The Teflon covered ion sources can be easily and quickly serviced without tools.

Using the Xcalibur™ data system package, the user can manage the PLATINblue system and the MSQ Plus – control, evaluation and report functions.

It just keeps runn

Fast and simple quantification
easy handling

The MSQ Plus mass detector supplies precise mass information for target analytes without the need for expert knowledge.

Groundbreaking features are the ESI and APCI FastLoc ion sources that allow the operating mode to be changed easily and quickly. The ion optic with patented cleaning of the sample inlet provides ultra-robust performance. Simple method development and sequence preparation is supported by templates. An automatic system autotune function and the calibration of mass range do not require the user to make any entries.

Versatile

Using the MSQ Plus mass detector, no compromises have to be made with regard to chromatography. The performance also remains robust when phases with ion pair reagents and non-volatile buffers are used or complex sample matrices are analysed. This mass detector's extremely wide range of applications covers standard HPLC through to UHPLC.

Ultra-fast scans

Scan speeds of 12000 amu/sec allow for fast data acquisition in shortest time for narrow peaks. In this way, the high throughput of the UHPLC can be used.

Unequalled flow rate range

From 10 µl/min to 2 ml/min in electrospray mode; from 200 µl/min to 2 ml/min in APCI mode.

ing!

Ionisation methods	Analytes
ESI: **Electro ionisation –** **gentle generation of ions under atmospheric pressure**	Preferred ionisation procedure for the analysis of biomolecules and smaller polar molecules. Typically, quasi-molecule ions are detected ($[M+H]^+$ for positive voltage; $[M-H]^-$ for negative voltage). Suitable for molecules up to 20000 m/z.
APCI: **Chemical ionisation** **at atmospheric pressure**	Depending on the solvent and analyte, reactions such as protonation, charge exchange, deprotonation and electron capture are possible. The method is not as careful as ESI; more fragment ions arise. Suitable for analytes with a molecular weight of up to 2000 m/z. For analytes that are poorly ionised using ESI, that only include a few reactive groups and that are thermally stable and vaporable.

Comparison of different single quadrupole mass spectrometers

	KNAUER MSQ Plus	Single Quad vendor 1	Single Quad vendor 2	Single Quad vendor 3
Ionisation techniques				
ESI sensitivity	50:1	50:1	100:1	50:1
ESI maximum flow rate (ml/min)	2	1	1	1
APCI ion source	included	optional	optional	optional
Specifications				
Mass range (m/z)	2 000	2 000	1 350	2 000
Max. scan speed (amu/s)	12 000	10 000	10 000	15 000
Width (cm)	30	35	40	35
Indicators				
Autotune software	✔	✔	✔	✔
Self-cleaning sample inlet, maintenance without tools	✔			

Easy to exchange

The FastLoc ion sources, the ion optic with automated cleaning function and the silently running vacuum system have been optimized to combine high speed with high sensitivity for an extremely high level of robustness.

FastLoc probes for quickly changing between ESI and APCI mode.

FastLoc ESI ion source

HPLC flow rates of capillary LC to conventional analytical LC (flow rates of 10 µl/min to 2 ml/min) without splitter

FastLoc APCI ion source

For all conventional HPLC columns with flow rates of 0.2 to 2 ml/min without splitter

Field-tested

The patented cleaning of the sample inlet maintains the performance of the mass detector even under the toughest conditions and reduces the amount of time-consuming and complicated cleaning steps. This is a procedure that is normally the case for LC/MS applications. The figure clearly shows that the critical part of the sample inlet is still clean even after 31 days of heavy-duty use with a phosphate buffer.

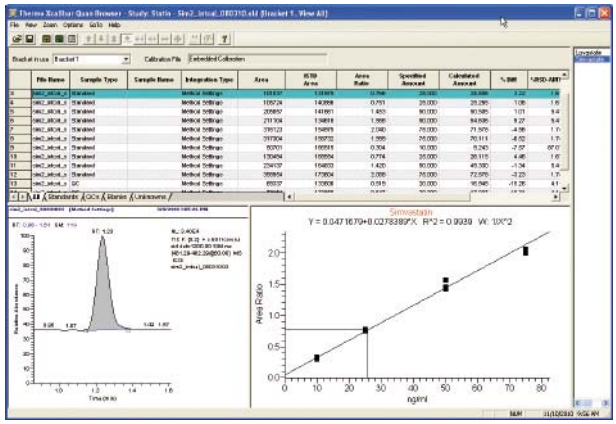
The software

Intuitive and comprehensive

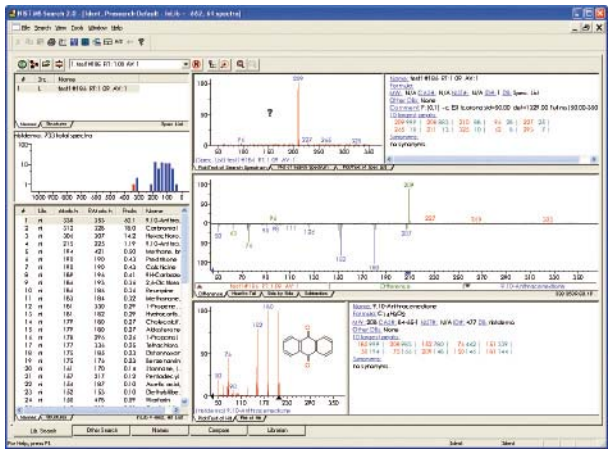
Using practical templates, even beginners can start immediately and develop methods and sequences.

The automatic calibration of the mass range and the autotune software function do not require any user entries.

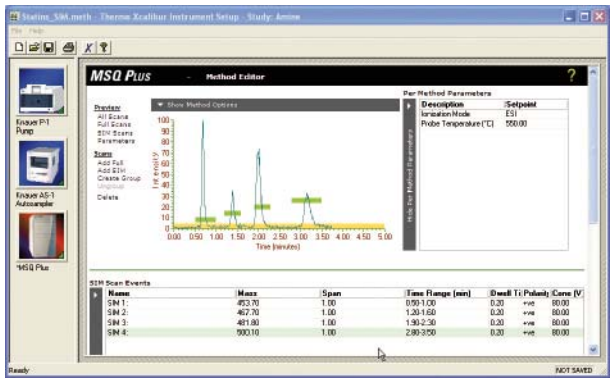
- 64 scans are possible for each method including the following options:
- Full scan and selected ion monitoring (SIM)
- Optional adjustable collision-induced dissociation (CID) in the ion source provides structural data
- Faster change of polarity for positive and negative ESI spectra from scan to scan
- With a single injection, scan and SIM data can be collected that enable the identification, verification and quantification of the target substances.
- The software complies with the requirements of 21 CFR Part 11, i.e. system security, multi-user options, implemented audit trails, electronic signatures and much more are included.



Quan browser: Here the results of the quantification can be reviewed, the parameters can be adjusted, new calibration data can be generated and analyzed samples can be quantified.



Library: The libraries module facilitates the creation of separate MS databases, the import of MS spectrum data from the Qual browser, the search for unknown substances, and the printing of reports.



In the method editor, the MS methods are created, i.e. scan mode (full scan or SIM) is defined with the respective operational parameters and the ionisation (ESI or APCI) as well as temperature are set.

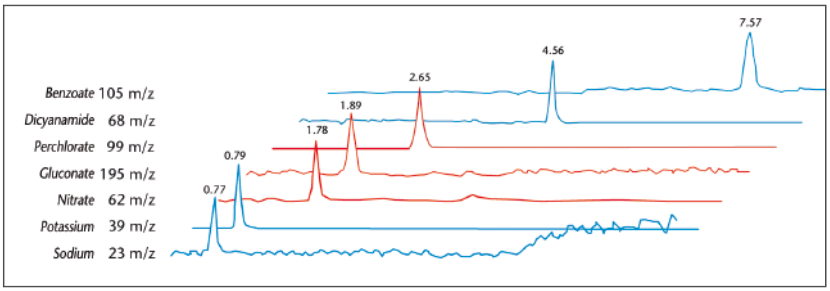
Qual browser: Here the spectra are evaluated, chromatographic peaks in the spectrum are optimized, ion masses and formulas are calculated, the spectra of unknown components are transferred to the library search, and spectra are exported to libraries.

The result

It can be this easy

Simplified ion analysis

The analysis of ions is greatly simplified using MSQ Plus. By quickly changing the polarity of the ESI mode, you can determine anions and cations in one run.

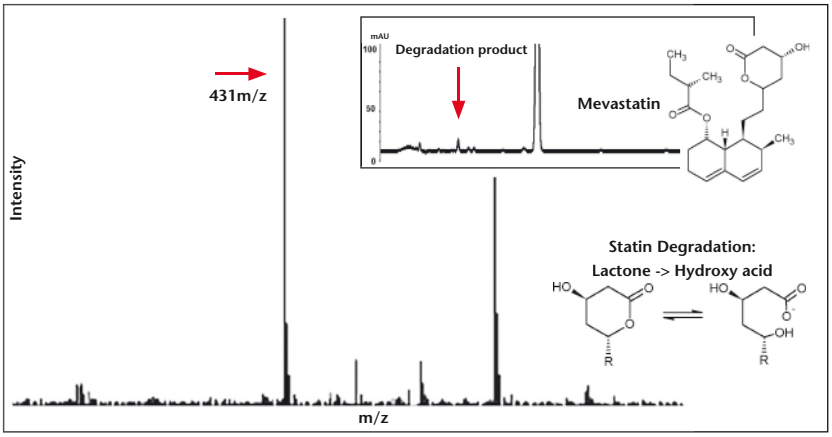


Separation conditions

Analyte	Anions and cations (see chromatogram)
Flow rate	0.3 ml/min
Mobile phase	Gradient. H_2O/MeOH, 1 % HCOOH
Injection volume	5 µl
Detector (MSQ)	ESI positive/negative mode
Capillary voltage	3.5 kV
Temperature	Ion source 350 °C

Identification of unknown compounds

The MSQ facilitates unique identification of impurities of an active substance when compared with conventional UV detection. A library search of the mass peak for m/z 431 finds a degradation product of Mevastatin. Opening the lactone ring forms the corresponding hydroxy acid.

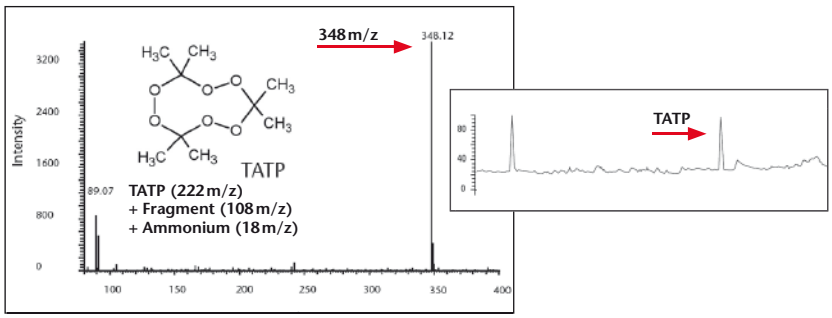


Separation conditions

Analyte	Mevastatin 100 mg/l
Flow rate	1.5 ml/min
Mobile phase	isocratic H_2O/ACN 35:65, 0.1 % HCOOH
Injection volume	10 µl
Detector (MSQ)	ESI positive
Capillary voltage	3.0 kV
Temperature	Ion source 550 °C

Detection of analytes that do not absorb UV

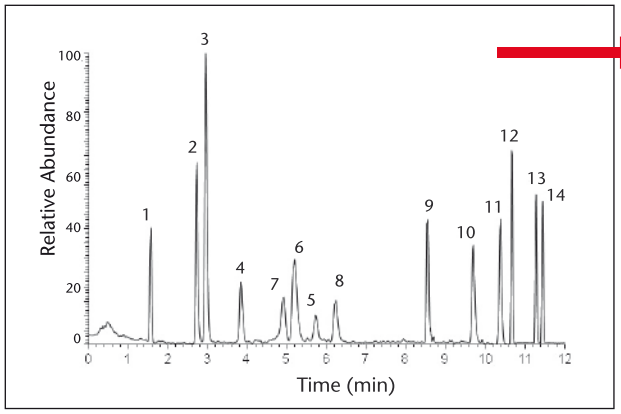
The analysis of highly explosive triacetone peroxide that, in contrast to most explosives, does not have any nitro groups, can be performed in a selective and sensitive manner using MSQ Plus.



Separation conditions

Analyte	Triacetone triperoxide (TATP)
Flow rate	0.5 ml/min
Mobile phase	binary gradient 1 mM ammonium formate/ methanol
Injection volume	2 µl
Detector (MSQ)	APCI positive
Corona	30 µA
Temperature	Ion source 350 °C

Multi-components determination of toxicologically relevant compounds

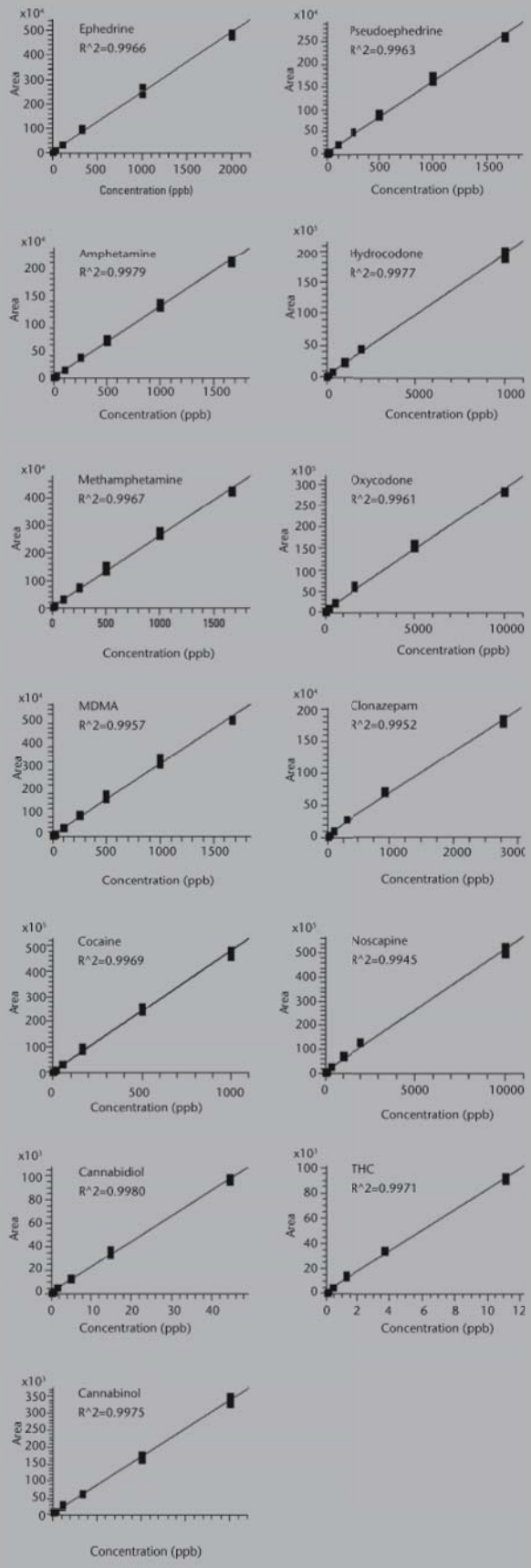


The MSQ Plus allows sensitive and robust quantification of a multi-component sample over a wide range of linearity. Compared with conventional detection using UV, the unique selectivity of lower limits of quantification and of detection are achieved for individual analytes.

Separation conditions

Analytes	see table
Mobile phase	ternary gradient H_2O/MeOH/ACN 0.1% acetic acid
Flow rate	1 ml/min
Injection	2 µl
Detector (MSQ)	ESI positive mode
Capillary voltage	4.5 kV
Temperature	Ion source 450 °C

	Analyte	Limit of quantification ng/ml	Limit of detection ng/ml	Linear ng/ml
1	Caffeine			
2	Ephedrine	1.21	0.36	1.3–2000
3	Pseudoephedrine	1.25	0.38	1.3–1670
4	Amphetamine	1.78	0.53	1.3–1670
5	Hydrocodone	6.80	2.04	4.1–1000
6	Methampheta-mine	0.96	0.29	1.3–1670
7	Oxycodone	3.48	1.04	3.3–10000
8	3.4-MDMA	1.09	0.33	1.3–1670
9	Clonazepam	7.39	2.22	3.3–3000
10	Cocaine	1.17	0.35	0.3–1000
11	Noscapine	3.79	1.14	0.7–10000
12	Cannabidiol	300	90.0	274–44400
13	THC	191	57.4	68.5–11100
14	Cannabinol	251	75.4	123–20000



Technical data

Mass spectrometer

MSQ Plus

Ionisation mode

- **ESI** Electrospray ionisation
- **APCI** Atmospheric-pressure chemical ionisation

Mass range

- 17 – 2000 m/z
  Optimized for scans of molecules in the low mass range

Scan speed

- Ultra-fast scan speed up to 12 000 amu/s

Sensitivity

ESI positive ionisation

- Mobile phase: acetonitrile/water at 1 ml/min
- Sample loop injection, 10 µl × 5 pg/µl erythromycin
- S/N: 50 pg erythromycin, 1000:1 RMS

ESI negative ionisation

- Mobile phase: methanol/water at 1 ml/min
- Sample loop injection, 10 µl × 2 pg/µl p-nitrophenol
- S/N: 20 pg p-nitrophenol, 500:1 RMS

APCI positive ionisation

- Mobile phase: acetonitrile/water at 1 ml/min
- Sample loop injection, 10 µl × 5 pg/µl erythromycin
- S/N: 50 pg erythromycin, 200:1 RMS

APCI negative ionisation

- Mobile phase: methanol/water at 1 ml/min
- Sample loop injection, 10 µl × 2 pg/µl p-nitrophenol
- S/N: 20 pg p-nitrophenol, 50:1 RMS

* Selected ion monitoring (SIM)

Installation requirements

Power supply

- Single phase, 230 V~, ±10 %, 50/60 Hz
- Distance to the next ground connection less than 2 m
- A power outlet for the MSQ Plus with a rated voltage of 15 A
- Minimum 3 power outlets with a total nominal current of 13 A (230V~)

Gas supply

- Pure, dry and oil-free nitrogen is required
- Minimum pressure 5 bar, required purity greater than 99 %
- A general nitrogen supply can be used as well as nitrogen gas generators specified for this
- The nitrogen supply must be able to supply 700 l/h
- In APCI mode under normal pressure, 450 l/h are required
- KNAUER offers a nitrogen gas generator (N418LA) that has been specially developed for the supply of LC/MS systems and generates a maximum 1080 l/h with the pressures needed for this and the required purity

Dimensions

- 300 x 530 x 710 mm (W x H x D)

Weights

- MS detector: approx. 60 kg
- Rotary pump: 45 kg typically standing on the floor
- Data system (including monitor): < 35 kg

Environment

- Max. heat dissipation in room 3 kW
- Ambient temperature must be stable between 15 °C and 35 °C
- Relative humidity between 40 % and 80 %
- No condensing water vapour
- The rotary pump should not be more than 1.5 m away from the instrument and should be accessible for maintenance
- An outlet is required for the waste gases of the ion source and the rotary pump
- The device should not be operated in the vicinity of strong magnetic fields such as those originating from NMR devices, high voltage power lines, transformers or mass spectrometers with a magnetic sector

Accessories: Nitrogen gas generator

Specifications

- Max. flow: 18 l/min (1080 l/h)
- Max. output pressure: 6.9 bar (100 psi)
- Particle size: < 0.01 µm
- Aerosols: No
- Phthalates: No

Design/setup

- Output: 1 x ¼" thread
- Internal air compressor: Yes, one
- Pressure gauge: Yes, one

Power supply

- 230V~, 50/60 Hz, 3.6 A

Dimensions

- 40 x 71 x 70 cm (W x H x D)

Weight

- 60 kg

Sleep mode function

- Reduces the runtime of the compressor and increases its life span

PLATINblue UHPLC

Specifications

- Flow rate: 0.01–5.0 ml/min (5 ml pump head)
- Max. pressure: 1000 bar (15000 psi) to 2 ml/min
  800 bar (11600 psi) to 5.0 ml/min
  (5 ml pump head)
- Flow rate accuracy: ± 1 %
- Flow rate precision: < 0.1%

PLATINblue HPLC Plus

HPLC Plus systems can be upgraded to complete UHPLC systems at any time.

- Flow rate: 0.01–10 ml/min
- Max. pressure: 750 bar (10880 psi) to 5 ml/min
  400 bar (5800 psi) to 10 ml/min
  (10 ml pump head)
- Flow rate accuracy: ± 1%
- Flow rate precision: < 0.1%

Order number	
A66500	MSQ Plus single quadrupole mass spectrometer
A69450	PLATINblue UHPLC/MS system
A66501	Nitrogen gas generator N418LA
A69420	PLATINblue UHPLC system, HPG, integr. degasser, PDA-1 detector, autosampler, column thermostat
A69420PH	PLATINblue HPLC Plus System, HPG, integr. degasser, PDA-1 detector, autosampler, column thermostat

Service

Fast and reliable

In order to maintain the high performance of your PLATINblue MSQ Plus for along time, we offer a service that guarantees smooth operation. Here we present the services that apply for the DE/AT/CH region. Please get in touch with your local KNAUER distributor to obtain a quote and discuss service options.

- Your personal PLATINblue MSQ contact partner is responsible for all service features
- On-the-job application advice – we support you during the running process with tips and tricks from our experience

- 1 year guarantee

- Installation service by your personal PLATINblue MSQ partner

www.platinblue.com

HPLC · SMB · Osmometry

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