JEOL

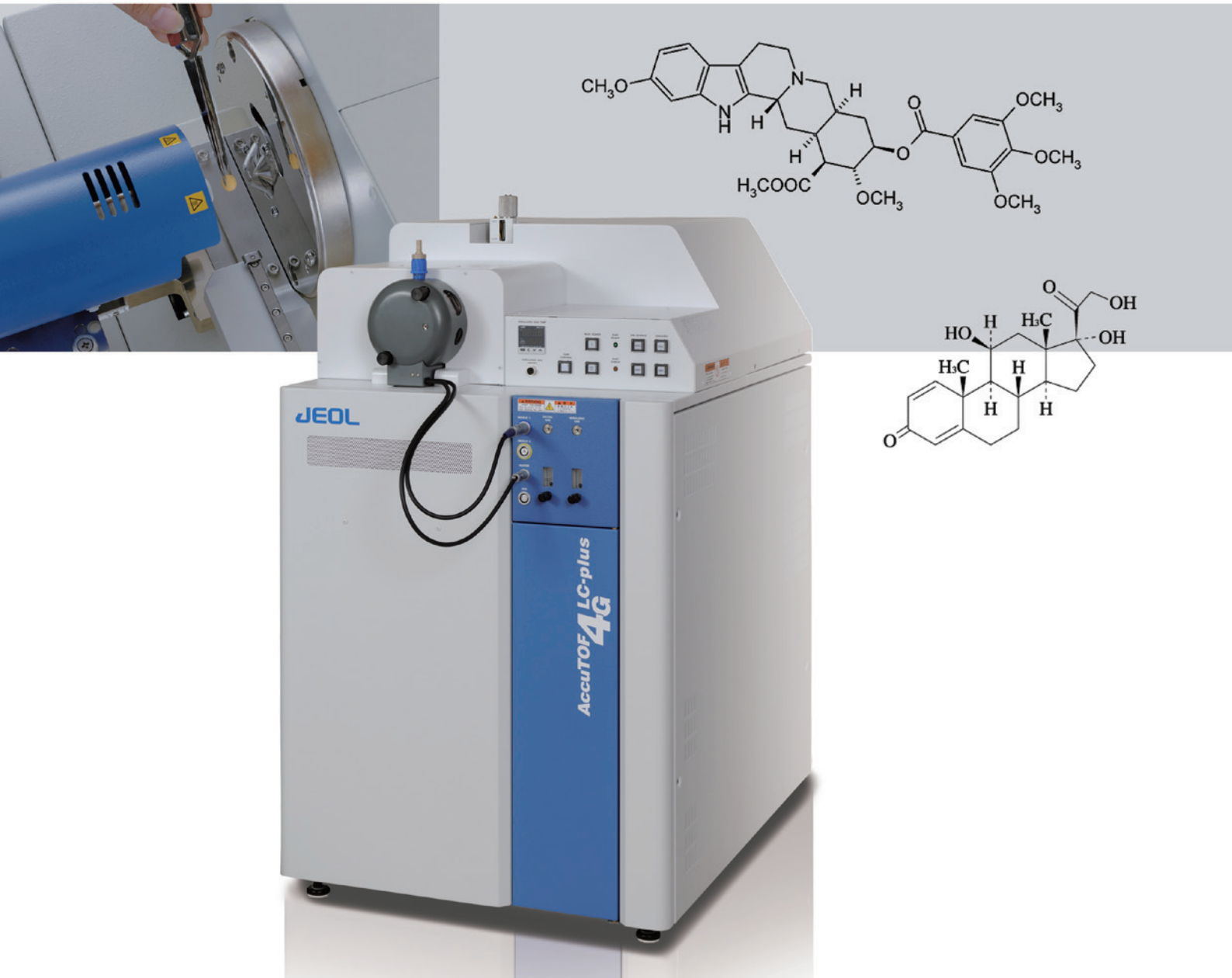
Scientific / Metrology Instruments

Atmospheric pressure ionization
high-resolution time-of-flight mass spectrometer

Solutions for Innovation

JMS-T100LP
AccuTOF LC-plus 4G

Simple, robust, and versatile atmospheric pressure ionization high-resolution time-of-flight mass spectrometer with variety of optional ion sources including DART and ColdSpray.



JEOL Ltd.

Simple, Robust, Versatile

AccuTOF LC-plus 4G

The AccuTOF LC-plus 4G, the third generation of the successful AccuTOF LC series, is a simple, robust and versatile atmospheric pressure ionization high-resolution time-of-flight mass spectrometer (API-HRTOFMS).
It can provide solutions for a wide variety of fields with JEOL's unique ionization technologies, DART and ColdSpray, in addition to the standard electrospray ionization (ESI), the most widely used ionization technique for LC/MS.

DART (Direct Analysis in Real Time)

DART mass spectrometer from the inventor of DART

With the optional DART ion source, samples with various states and shapes can be analyzed directly without any sample preparation.
DART was born in 2003 at the mass spectrometry applications laboratory of JEOL USA, Inc. Among a series of new ionization techniques, which were late termed "ambient ionization," DART was the first to be invented and the first to be commercialized in 2005.

LC/MS

The AccuTOF LC-plus 4G is a simple and robust LC/MS system. It offers a wide variety of applications for LC/MS with optional Atmospheric Pressure Chemical Ionization (APCI) source, in addition to the standard orthogonal ESI source. Accurate mass measurements in LC/MS can be made routine by automating the introduction of the internal mass reference compound with the optional Auto-Injection Valve.

ColdSpray

With the optional ColdSpray ion source, thermally labile analytes, including self-assembling supra molecules, some classes of organometallic complexes, short-chain double stranded DNAs, can all be analyzed intact.
ColdSpray ionization was developed by Prof. Kentaro Yamaguchi, et al., of Kagawa School of Pharmaceutical Sciences, Tokushima Bunri University (previously Chiba University) and the result of a project funded by the Japan Science and Technology Agency (JST).

Proven performance

The AccuTOF LC-plus 4G delivers reliability through innovation.

Advanced performance

High-frequency, high-voltage RF ion guide

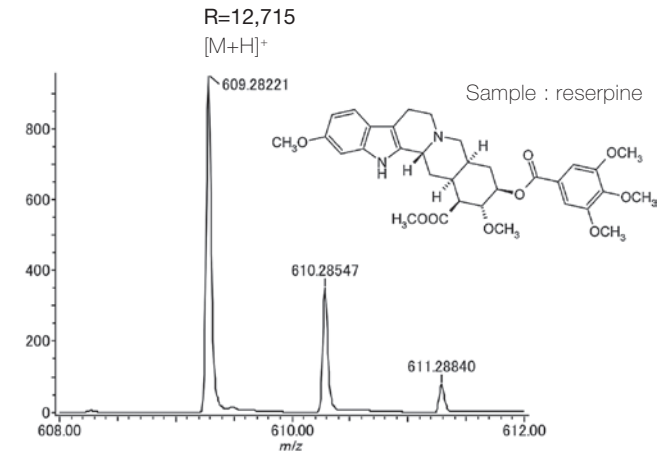
Ions with low *m/z* can be readily observed with an unique high-frequency, high-voltage RF ion guide.
The operating condition of the DART ion source can be easily diagnosed by monitoring atmospheric ions such as protonated water dimer [$(H_2O)_2$ + H]$^+$ (*m/z* 37), oxygen anion O_2^- (*m/z* 32), etc.

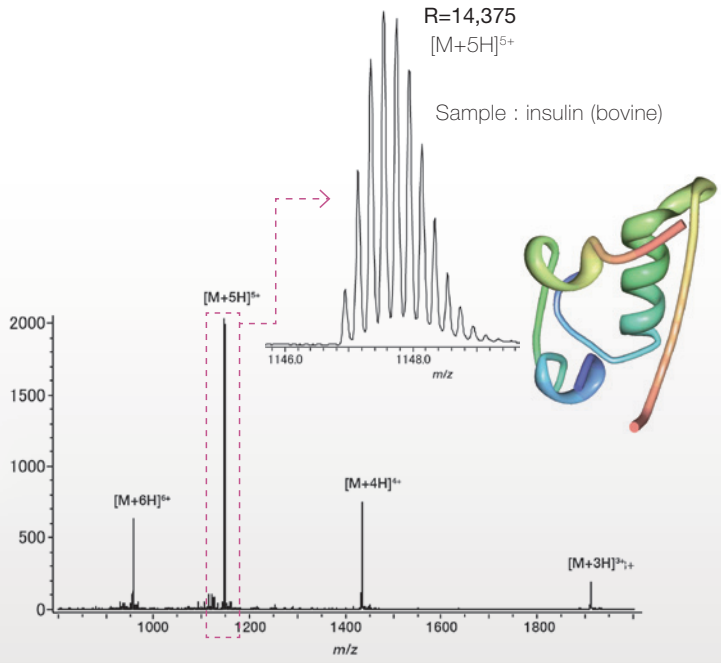
High response detector

High speed and high sensitivity micro channel plate (MCP) detector unit.

High speed digitizer

High speed data recording (up to 50 spectra/s) and wide dynamic range have been realized with 4 gigasample/s high-speed digitizer (ADC) and a high-performance data acquisition system.





Robustness / Easy Maintenance

Vacuum isolation valve

The ion transport region can be cleaned or maintained without breaking the high vacuum of the time-of-flight mass analyzer.
Very little downtime is required for routine maintenance.

Simple and robust ion sources

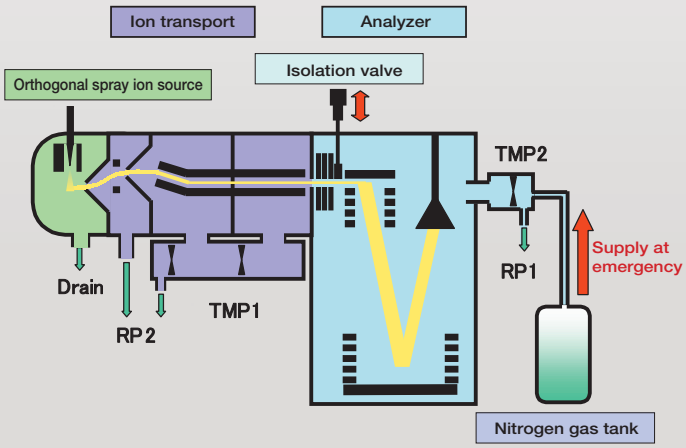
A simple design supports easy maintenance. The API interface is contamination resistant to handle a variety of samples and analyses. Ion sources, including DART and ESI can be easily exchanged.

Nitrogen gas tank

The mass analyzer vacuum chamber is automatically purged with nitrogen gas stored in the gas ballast tank when the system is stopped, even for an accidental and/or unexpected power outage. This protects the oxygen- and moisture-sensitive MCP detector and reduces the vacuum pump-down time.

Robust, high-capacity vacuum pumping system

The DART source is commonly operated with helium.
The AccuTOF LC-plus 4G is the only atmospheric-pressure ionization mass spectrometer systems that can pump helium without any additional hardware.



* Image of RCSB PDB (www.rcsb.org) ID 4IHN (Pechkova, et al., A Review Of The Strategies For Obtaining High Quality Crystals Utilizing Nanotechnologies And Space) created with Protein Workshop (Moreland, et al. (2005) BMC Bioinformatics 6:21).

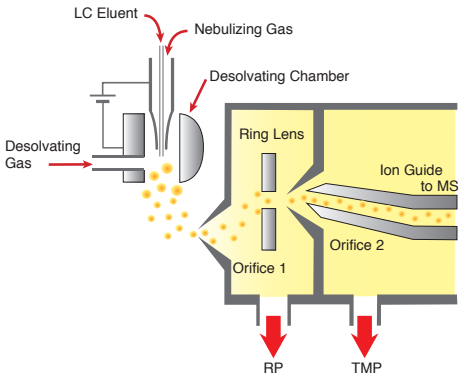
Simple, Robust, Versatile

Robust LC/MS system

Robust hardware

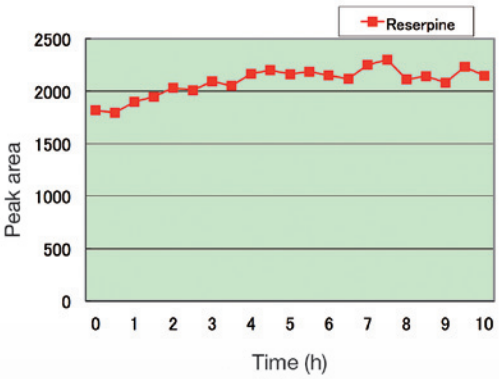
Orthogonal electrospray ion source, off-axis orifices and bent ion guide prevents contamination to the mass analyzer.
Required daily maintenance is simply involves wiping orifice 1 clean.

Schematics of the orthogonal electrospray ion source



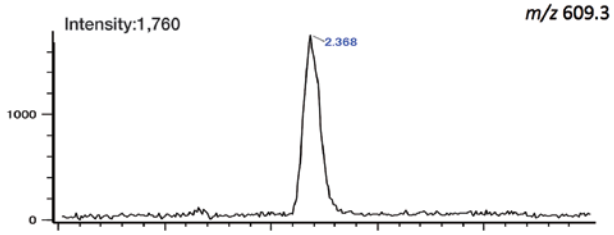
Durable, contamination-resilient ion source

Helps minimizing down time and maintains stable sensitivity for longer periods of time.

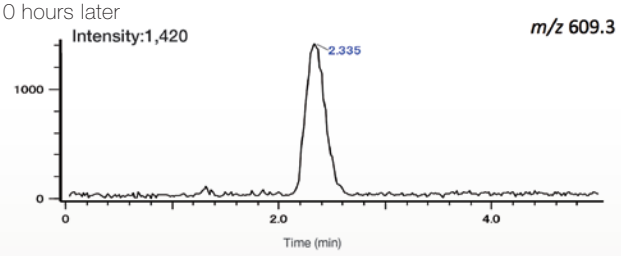


Reserpine standard was analyzed repeatedly for 10 hours with gradient elution by 5 mM phosphate buffer / acetonitrile.

Measurement start



10 hours later



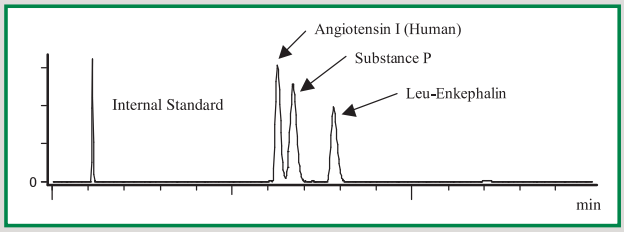
Automated introduction of internal mass reference compound

An Internal mass reference compound is necessary for performing accurate mass measurements with the highest mass accuracy. However, manually introducing mass reference compounds for every analysis is cumbersome, especially when analyzing a large number of samples.
The Auto-Injection Valve* can automate the introduction of the mass reference compound, making the accurate mass measurements routine. The timing of the introduction can be set within the data system software.

* Optional Auto-Injection Valve

Accurate mass measurement of a peptide mixture with Auto-Injection Valve

Total ion current chromatogram of the peptide mixture



Accurate mass measurement result

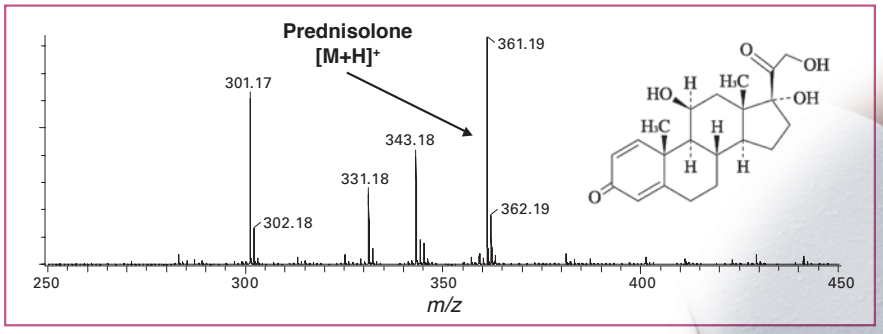
	Calculated *(m/z)*	Measured *(m/z)*	Err. (mDa)	Err. (ppm)
Angiotensin I (Human)	1296.68531	1296.68544	0.13	0.10
Substance P	1347.73597	1347.73752	1.55	1.15
Leu-Enkephalin	556.27712	556.27731	0.19	0.33

DART (Direct Analysis in Real Time)

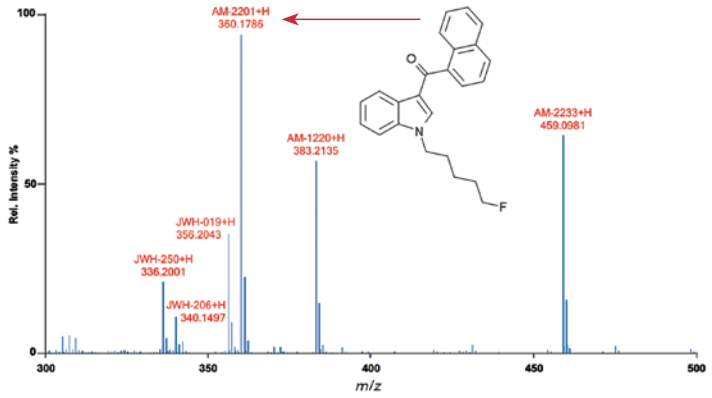
JEOL, the pioneer of ambient ionization

DART was born in 2003 at the mass spectrometry applications laboratory of JEOL USA, Inc. Among a series of new ionization techniques, which were later termed “ambient ionization,” DART was the first to have been invented and the first to have been commercialized in 2005. It was introduced at the Pittsburgh Conference in February 2005 and awarded the Pittcon Editors’ Gold Award as one of the best new products of the year. It was also awarded for the R&D 100 Award in September of the same year.

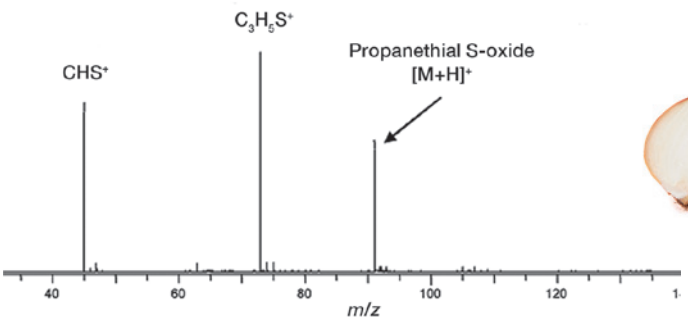
Steroid tablet Held between tweezers



Designer drug (synthetic cannabinoids)



Lachrymator detected from freshly chopped chive bulbs

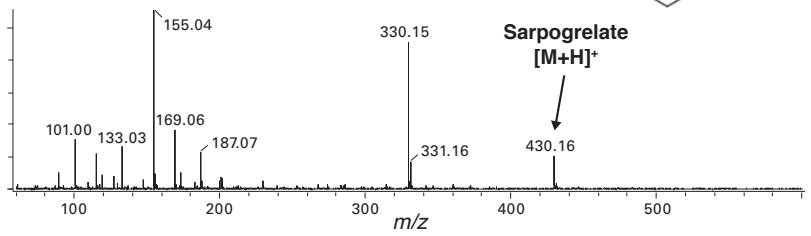


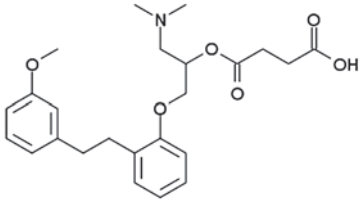
Direct analysis without sample preparation

You can acquire high mass-resolution, accurate mass spectra in real time by simply presenting samples of various shapes and states to the DART ion source without any sample preparation.
DART can handle samples with arbitrary shapes or “dirty” sample that conventional analytical method cannot deal with.

Robust

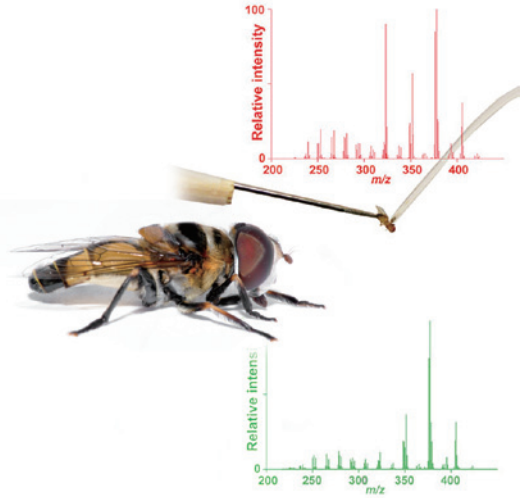
Antithrombotic drug (liquid) At the tip of a glass rod





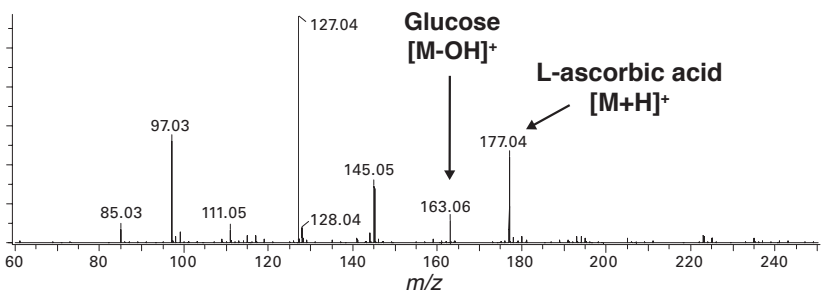
Sarpogrelate [M+H]⁺

Fruit fly pheromone



Data courtesy of Dr. Joanne Yew (Temasek Life Sciences Laboratory, Singapore – previously Harvard Medical School)

Vitamin-C granules (dietary supplement) Powder wrapped in a ceramic sheet

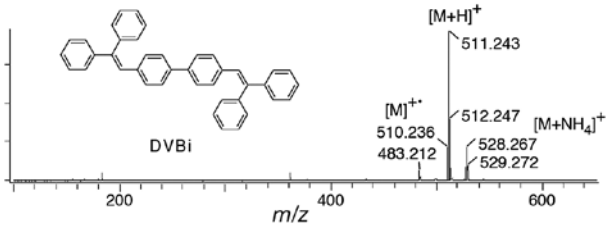


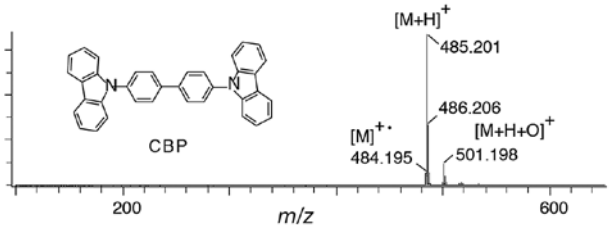
DART (Direct Analysis in Real Time)

AccuTOF LC-plus 4G + DART: the perfect combination

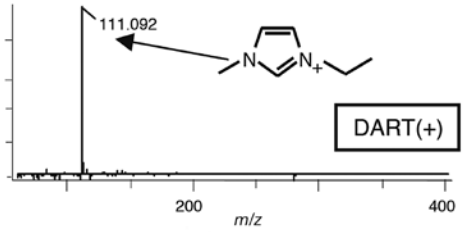
The DART was developed for the JEOL AccuTOF series of mass spectrometers. No additional interface is required between the DART and the AccuTOF LC-plus 4G due to a rugged, simple API interface and high-capacity vacuum pumping system. The combination is able to detect a wider range of polar and nonpolar compounds than any other DART MS system. With no additional interface, there is virtually no carryover from one analysis to another, even for “dirty” and “sticky” samples.

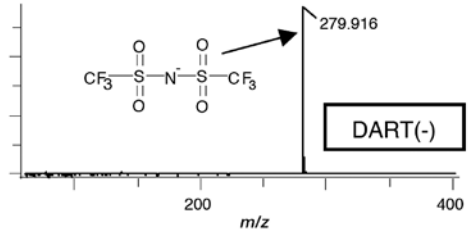
Nonpolar: organic electroluminescence materials





Polar: an ionic liquid



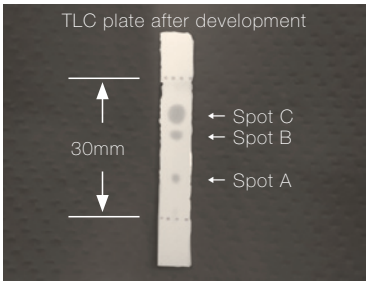


Direct analysis of a TLC plate

Sample: over-the-counter cold medicine

Sample extraction: chloroform
Developing solvent: chloroform/methanol = 9/1

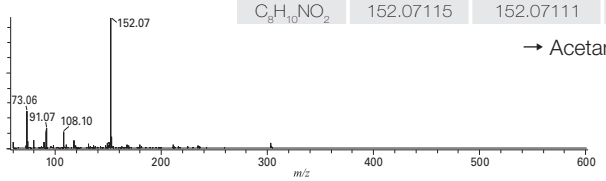
Mass spectrum and accurate mass measurement result from each spot are shown on the right.



Spot A (*m/z* 152)

Formula	Calc. (*m/z*)	Meas. (*m/z*)	Err. (mDa)
$C_8H_{10}NO_2$	152.07115	152.07111	-0.04

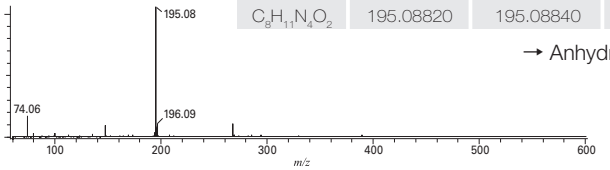
→ Acetaminophen



Spot B (*m/z* 195)

Formula	Calc. (*m/z*)	Meas. (*m/z*)	Err. (mDa)
$C_8H_{11}N_4O_2$	195.08820	195.08840	0.20

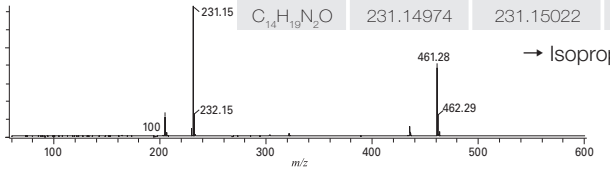
→ Anhydrous Caffeine



Spot C (*m/z* 231)

Formula	Calc. (*m/z*)	Meas. (*m/z*)	Err. (mDa)
$C_{14}H_{19}N_2O$	231.14974	231.15022	0.48

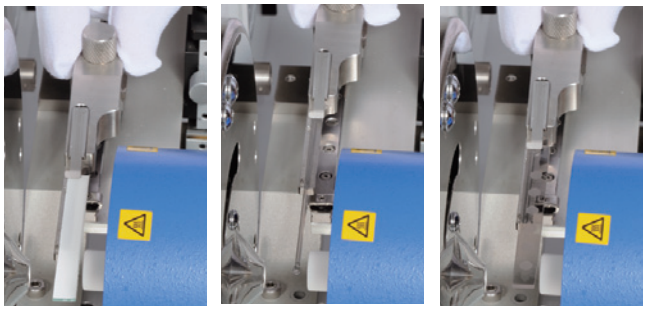
→ Isopropylantipyrine



Wide variety of sample introduction options

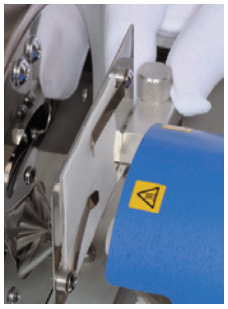
TLC Sampler

In addition to a TLC plate cut into a strip, a glass rod with liquid sample at the tip and a glass sample plate with indented sample spots can be introduced.



Sheet Holder

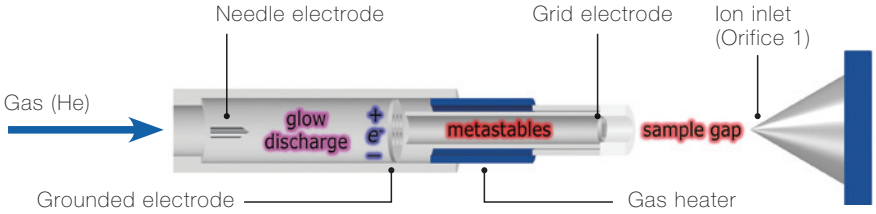
To introduce powder samples wrapped in a ceramic sheet.



TLC Autoslider

A glass TLC plate cut into a strip can be moved through the gap with constant velocity.

Principle of DART ionization



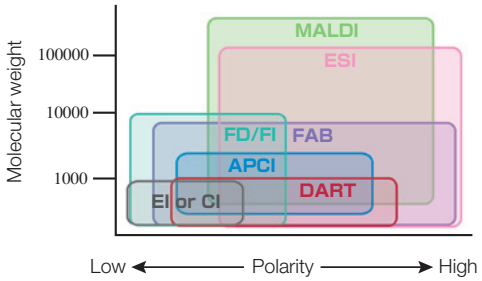
DART ionization is based on the interaction between excited state atoms or molecules, and atmospheric gas and/or analytes. Plasma is generated by glow discharge from the needle electrode in a helium gas stream. The plasma includes ions, electrons, and excited state (metastable) atoms or molecules. The majority of charged particles are eliminated by the grounded electrode and the excited state neutral species are expelled to the atmosphere.
The gas stream can be heated by the gas heater to help analytes vaporization or desorption from the substrate surface.

■ Positive ion

The metastable helium atoms formed in the DART source react with atmospheric water to produce ionized water clusters. These protonated water clusters can then react with the analyte (M) to form protonated cations:

$$He(2^3S) + H_2O \rightarrow H_2O^{+\cdot} + He(1^1S) + e^-$$
$$H_2O^{+\cdot} + H_2O \rightarrow H_3O^+ + OH^\cdot$$
$$H_3O^+ + nH_2O \rightarrow [(H_2O)_{n+1} + H]^+$$
$$[(H_2O)_{n+1} + H]^+ + M \rightarrow [M + H]^+ + (n+1)H_2O$$

Application range of each ionization method



■ Negative ion

Metastable helium atoms can react with a neutral (N), such as the exit grid electrode, or another neutral species to form electrons through Penning ionization. The electrons formed are rapidly thermalized by collisions with atmospheric gases (G) and then react with gaseous oxygen to produce oxygen anions.

$$He(2^3S) + N \rightarrow N^{+\cdot} + He(1^1S) + e^{-\cdot}$$
$$e^{-\cdot} + G \rightarrow G^* + e^-$$
$$e^- + O_2 \rightarrow O_2^{-\cdot}$$

These oxygen anions can then react with sample molecules (M) to produce analyte anions.

$$O_2^{-\cdot} + M \rightarrow [M - H]^- + OOH^\cdot$$
$$O_2^{-\cdot} + M \rightarrow M^{-\cdot} + O_2$$
$$O_2^{-\cdot} + M \rightarrow [M + O_2]^{-\cdot}$$

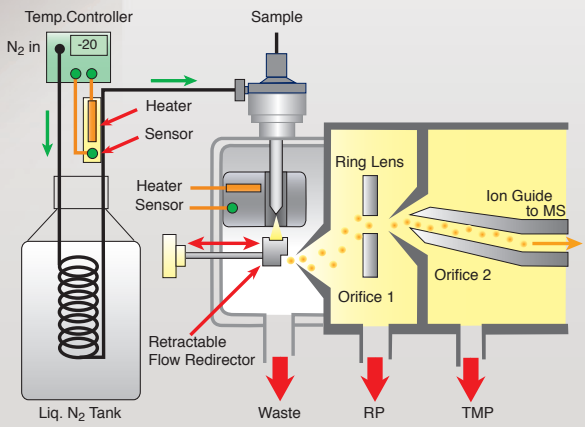
Towards even softer ionization

Analysis of supramolecules and noncovalently bound complexes

Supramolecules and organometallic complexes ~ ColdSpray

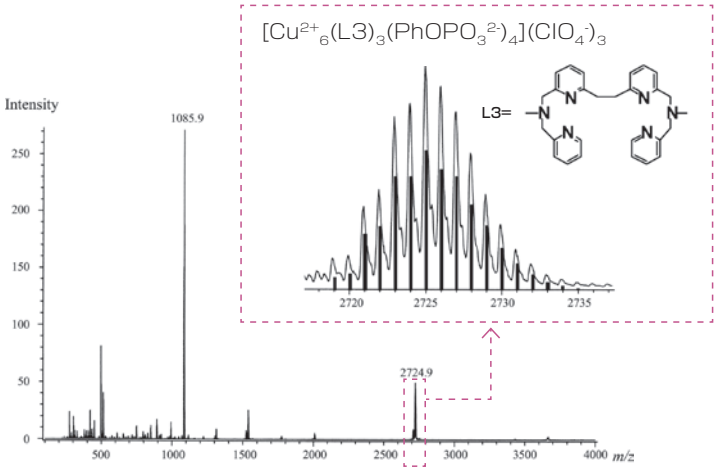
The ColdSpray ion source facilitates the analysis of very unstable species that are difficult to analyze by electrospray. The applications of ColdSpray have been expanding from organometallics complexes to unstable reaction intermediates, host-guest complexes, clusters in solution, and biomolecules.

Schematics of the ColdSpray ion source

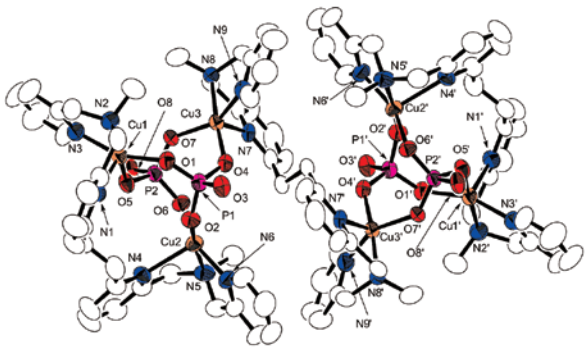


ColdSpray ionization was developed by Prof. Kentaro Yamaguchi, et al., of Kagawa School of Pharmaceutical Sciences, Tokushima Bunri University (previously Chiba University) and the result of a project funded by the Japan Science and Technology Agency (JST).
Reference: Cold-Spray ionization mass spectrometry: principle and applications K. Yamaguchi, J. Mass Spectrom, 38, 473-490 (2003)

ColdSpray mass spectrum of a hexanuclear copper complex in acetonitrile at -30℃



ORTEP diagram of the complex [Cu2+6(L3)3(PhOPO3 2-)4]

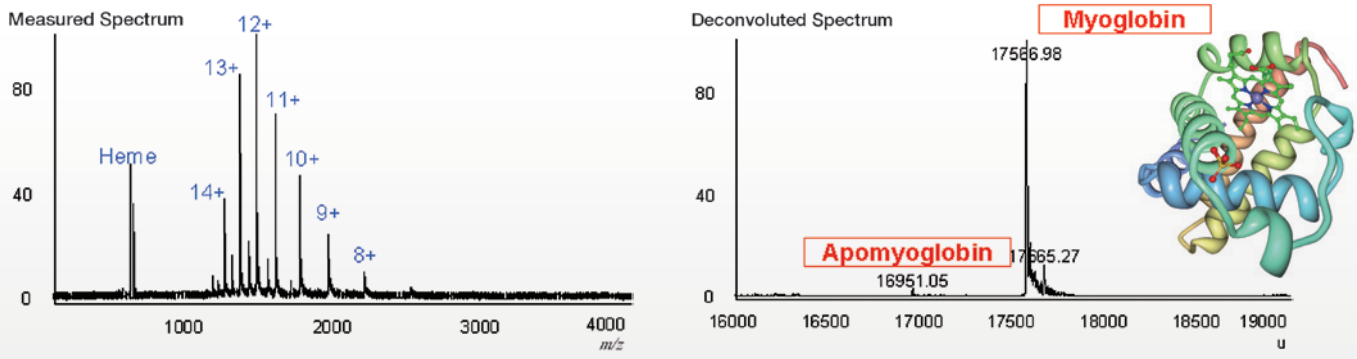


(Data courtesy of Prof. Masahito Kodera, Doshisha University)

Heme proteins ~ Nano ESI

Nano ESI achieves efficient desolvation with a minimum amount of heat by performing electrospray at very low flow rates. Myoglobin, a heme protein with noncovalently bound heme, was analyzed intact.

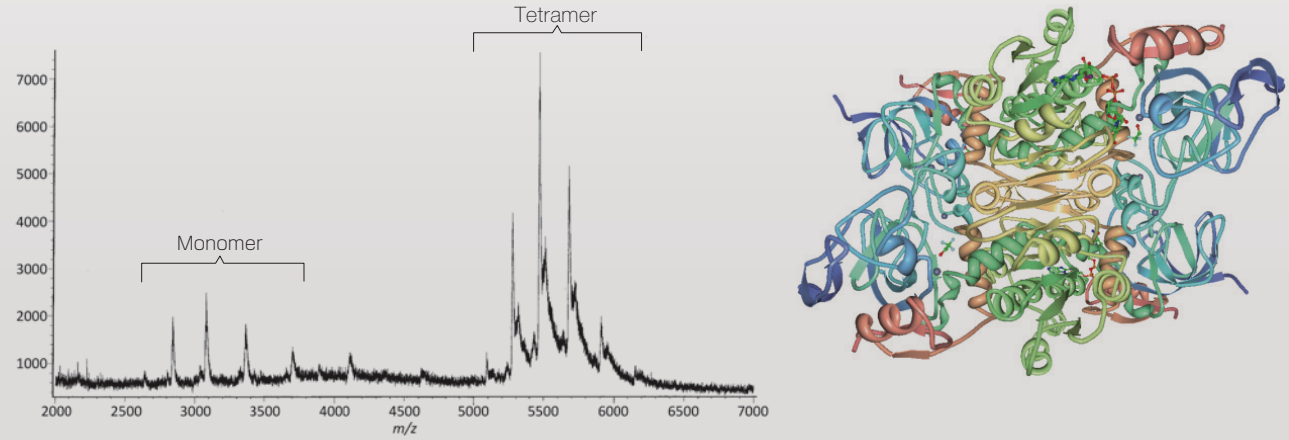
Nano ESI mass spectrum of myoglobin (equine heart)



Protein complexes ~ adjustment of interface pressure

Protein complexes, which are difficult to detect intact, can be analyzed by adjusting the vacuum pressure between the Orifice 1 and Orifice 2 with an optional vacuum adjustment valve.

ESI mass spectrum of alcohol dehydrogenase complex (yeast)



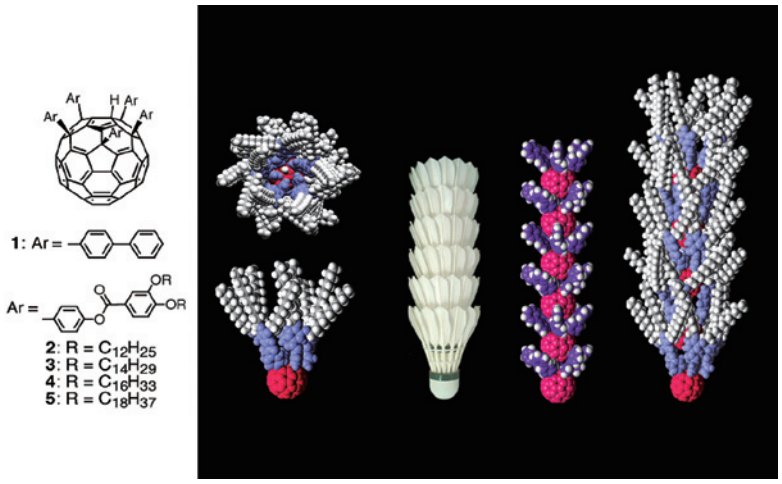
* Image of RCSB PDB (www.rcsb.org) ID 4IHN (Maurus, et al. (1997) Biochim.Biophys.Acta 1341: 1-13) created with Protein Workshop (Moreland, et al. (2005) BMC Bioinformatics 6:21).
* Image of RCSB PDB (www.rcsb.org) ID 4W6Z (Raj, et al. (2014) Biochemistry 53: 5791-5803) created with Protein Workshop (Moreland, et al. (2005) BMC Bioinformatics 6:21).

Ever expanding applications

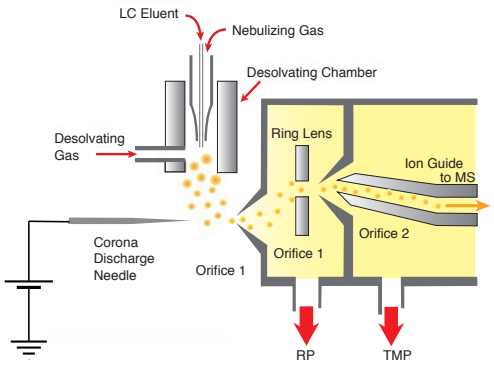
Analysis of nonpolar, high molecular weight compounds

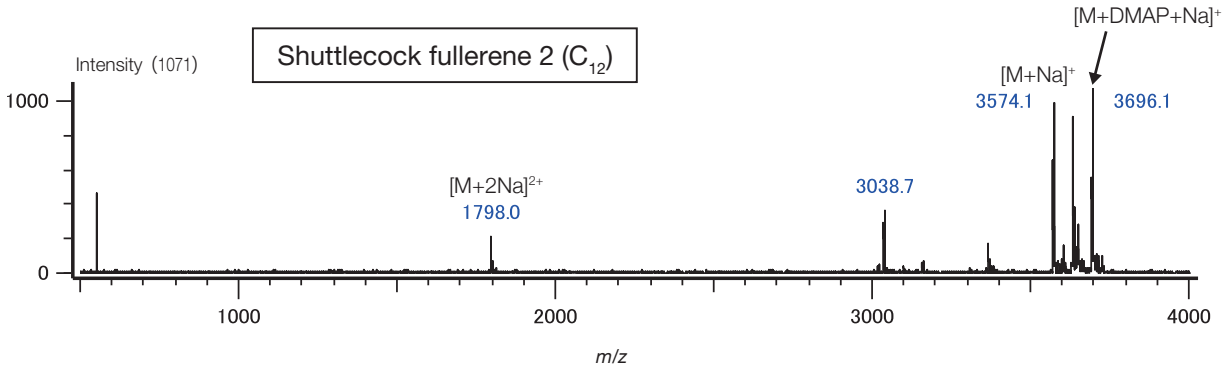
Fullerene derivatives ~ Atmospheric Pressure Chemical Ionization (APCI)

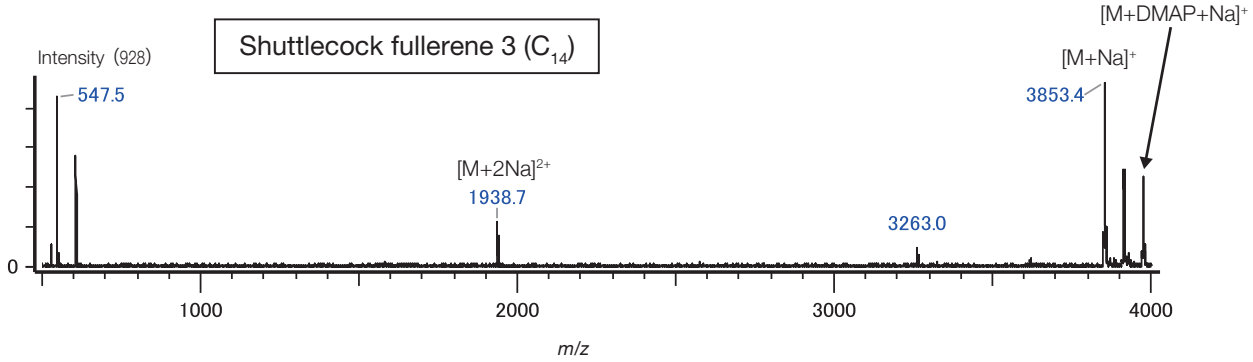
"Shuttlecock fullerenes," which are nonpolar and high molecular weight (MW > 3,000) were analyzed with an optional APCI ion source.



Schematics of the orthogonal APCI ion source







(Samples courtesy of Prof. Eiichi Nakamura, The University of Tokyo)

Easy maintenance

Easy and quick ion source exchange

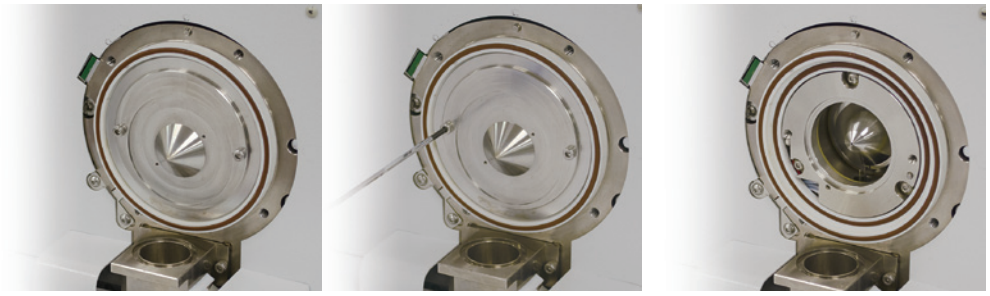
Switching from ESI to DART is easy and quick on AccuTOF LC-plus 4G since no additional interface for DART needs to be installed.

1 ·····► 2 ·····► 3 ·····► 4

Easy and quick interface cleaning

Daily cleaning is as simple as wiping off the outside of Orifice 1.
When analyzing self-assembling supramolecules by ColdSpray, often the sample concentration has to be quite high in order to promote the formation of the supramolecules. You will have to clean the inside of the Orifice 1 after such analyses. For the AccuTOF LC-plus 4G equipped with the isolation valve, downtime for cleaning beyond Orifice 2, even wiping clean the ion guide, can be done in minutes, not hours.

1 ·····► 2 ·····► 3 ·····►

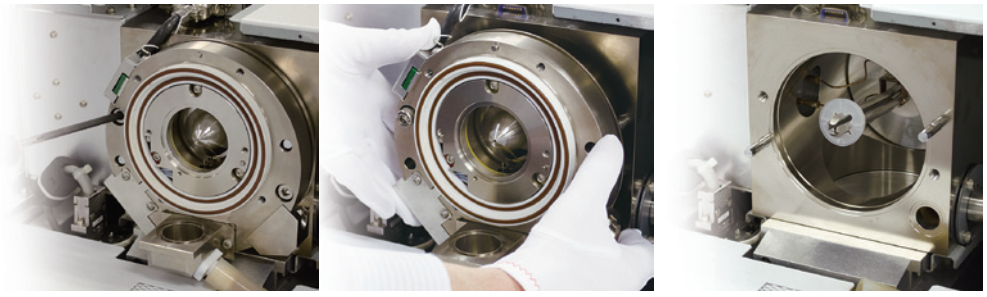


Daily maintenance is simply involves wiping Orifice 1 clean.

If you need to clean inside, remove Orifice 1…

Clean the back side of Orifice 1, Ring Lens, and front side of Orifice 2.

4 ·····► 5 ·····► 6



Remove Orifice 2…

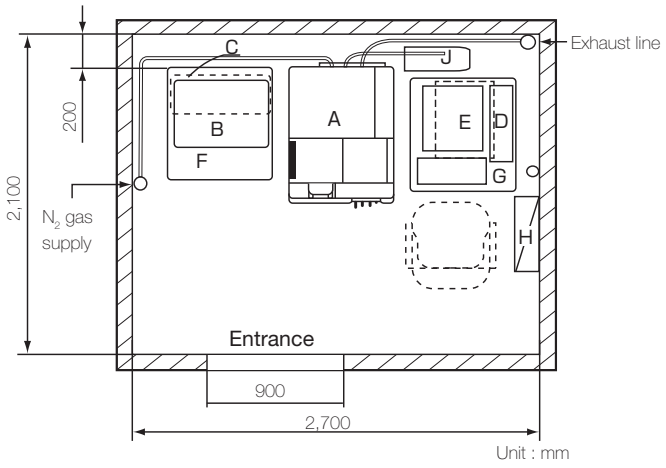
Clean the back side of Orifice 2 and Ion Guide.

Installation requirements

Power supply	
Main console	Single phase AC 190-210 V or 220-140 V, 50-60 Hz, 30 A*
Liquid chromatograph	Single phase AC 100-120 V, 20 A or 200-140V, 10 A*
DART ion source	
Data system	Single phase AC 100-120 V, 15 A or 200-140 V, 7.5 A*
Grounding	100 Ω or less
Nitrogen gas	
Main console	700 kPa（10 L/min）, 97 % or better purity
DART ion source	550 kPa（10 L/min）, 97 % or better purity
Helium gas	
DART ion source	550 kPa（10 L/min）, 99 % or better purity
Installation room	
Varying magnetic field	1×10^{-6} T or less
Static magnetic field	5×10^{-4} T or less
Floor vibration	Amplitude (p-p) 25 μm or less, acceleration 0.1 m/s 2 or less
Room temperature	20 ~ 27 ˚C
Temperature fluctuation	± 3°C /h or less
Humidity	30 to 70% (no condensation)
Maximum heat generation	28,800 kJ/h with liquid chromatograph
Ventilation facility	Ventilation facility for solvent vapor (from ion source) and rotary pumps is required.

* Power supply requirement depends on a specific configuration sold in each territory. Please inquire at a local sales office for details.

Example of an installation room (with liquid chromatograph)



	Unit	W (mm)	D (mm)	H (mm)	Mass (kg)
A	Mass spectrometer	690	905	1156	305
B	Liquid chromatograph	620	435	900	49
C	N_2gas tank	250	660	170	15
D	Computer	172	471	414	14
	LCD monitor	510	180	390	3
E	Laser printer	385	279	261	6
F	Table for LC	-	-	-	-
G	Table for PC	-	-	-	-
H	Switch board	-	-	-	-
I	N_2 gas supply -	-	-	-	
J	Rotary pump	160	430	230	22

*Specifications subject to change without prior notice.

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