![JEOL — Solutions for Innovation]

Solutions for Innovation

JMS-Q1600GC
UltraQuad™ SQ-Zeta

JEOL Ltd.

"Zeta"
The 6th generation high-end GC-QMS is finally here!

The new JMS-Q1600GC UltraQuad™ SQ-Zeta of JEOL is our 6th generation high-end Gas Chromatograph Quadrupole Mass Spectrometer (GC-QMS) based on JEOL's 50 years of MS technologies and experience.

From quantitative applications such as environmental samples, water quality control and agrochemicals, to qualitative applications such as materials and aroma analyses, the SQ-Zeta is the ultimate general-purpose GC-MS with high-performance capabilities for a wide variety of measurement and analysis needs.

JMS-Q1600GC UltraQuad™ SQ-Zeta
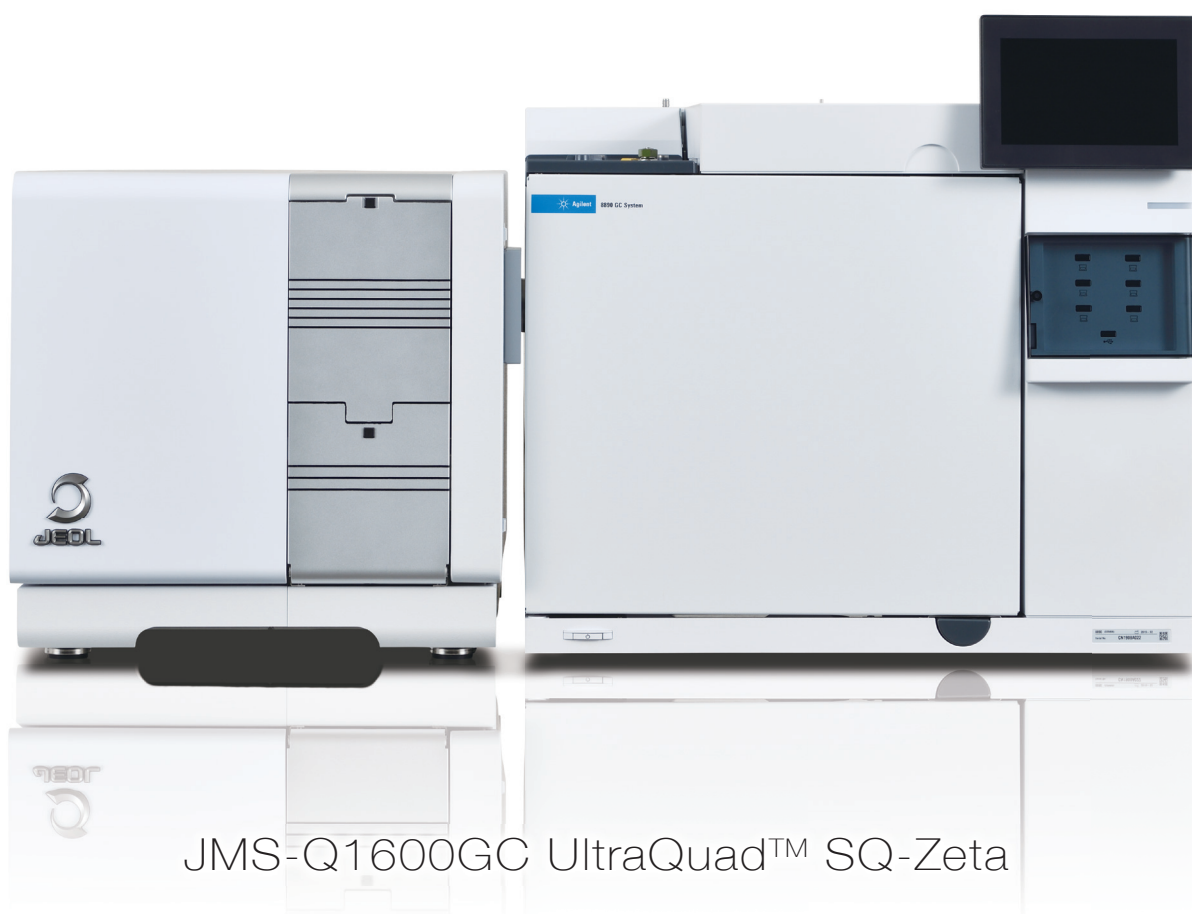
Genealogy of Benchtop Quadrupole Mass Spectrometer by JEOL

2003

JMS-K9

· First generation JEOL GC-QMS
· Large Dipole electrode, Large TMP adopted
· Novaspec software

2005

JMS-Q1000GC

· Scan sensitivity: Highest in class
· Escrime™ software for quantitative analysis
· EI ion source for high concentration sample analysis

2008

JMS-Q1000GC MkII

· Scan sensitivity: Further improved
· Applicable to JEOL headspace sampler

2011

JMS-Q1050GC

· Filament with long durability
· Dual filaments employed
· Photoionization source introduced

2016

JMS-Q1500GC

· Newly-designed control circuit and MSPRIMO™ software
· Integration of qualitative/quantitative analysis into the Escrime™ software
· Draw-in Lens added

JEOL mass spectrometer development started with the magnetic sector mass spectrometer JMS-01, which was launched in 1963. In the 1970's, we began doing fundamental research into quadrupole mass spectrometers (QMS). In 1972, JEOL officially launched the JMS-Q10, a high-performance GC-QMS equipped with large-sized quadrupoles (hyperbolic-shaped electrodes). With the launch of JMS-AM Series AUTOMASS in 1989, JEOL made a full-fledged entry into the QMS market. In 2003, JEOL introduced its long-awaited successor GC-QMS, the JMS-K9. The JMS-K9 was equipped with a large-sized hyperbolic-shaped electrode and a high-capacity TMP. This system was built on the concept of the AUTOMASS but upgraded with the latest circuit technology and computer system. Since 2003, the JMS-K9-based system and hardware have been continuously upgraded, leading to the release of the 5th generation GC-QMS into the market (JMS-Q1500GC) in 2016. Now JEOL has introduced the 6th generation GC-QMS, the JMS-Q1600GC UltraQuad™ SQ-Zeta. The SQ-Zeta succeeds the technologies that were cultivated in its predecessors with additional upgraded functionality. The new JMS-Q1600GC UltraQuad™ SQ-Zeta represents a step into the future for all of your GC-QMS analytical needs.

High Performance Advantage
Advanced mass spectrometry technologies brought together

The JMS-Q1600GC UltraQuad™ SQ-Zeta is equipped with the largest hyperbolic-shaped quadrupole in its class. The hyperbolic design allows two features: wide dynamic range from much larger ion volume, and high sensitivity due to superb ion transmission.

Front

High-precision Hyperbolic-shaped Quadrupole
· Superb ion transmission enhances high sensitivity
· Reduces ion-quenching when introducing a large volume of ions, allowing a wide dynamic range

Pre-filter
· Suppresses the degradation of resolution and sensitivity due to contamination of the quadrupole

Dual Filament
· Reduces instrument down-time during filament exchange

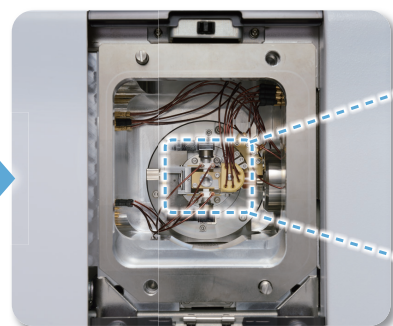# No tools required
Easy maintenance!

No tools are required to remove or insert the ion source chamber.
As with previous models, a large ion source flange is used to ensure ease of access.
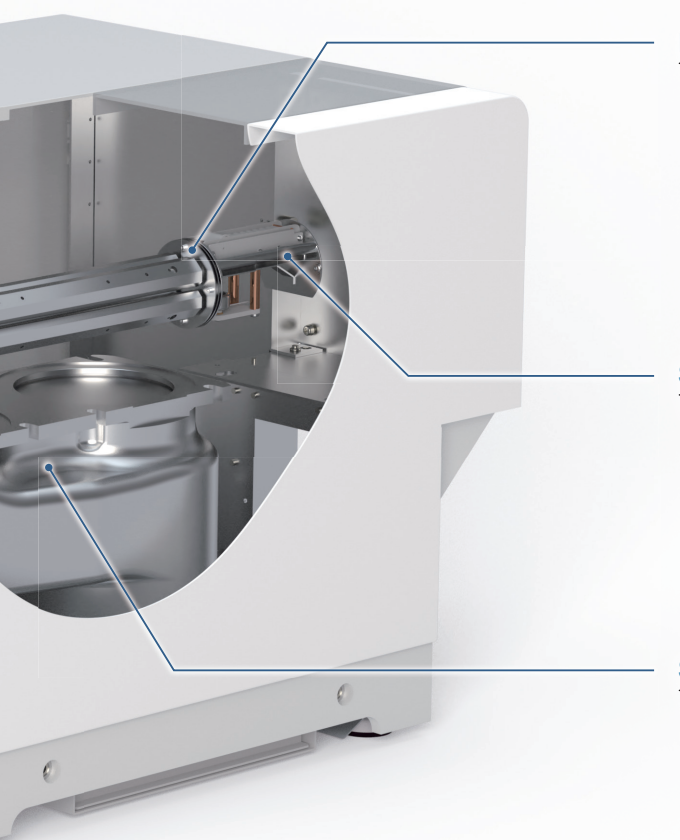
1. Remove the cover.

2. Remove the flange.

Draw-in Lens

· Reduces diffusion of ions from the quadrupole outlet and reduces chemical noises
· Improved sensitivity by re-acceleration of ions

Secondary Electron Multiplier Detector

· Detector is resistant to degradation in an atmospheric environment to maintain high performance over a long period of time

Split Flow Turbo Molecular Pump

· Quick evacuation after column replacement and maintenance work
· Use of mega bore, packed column is possible
· Compatible with the latest Low-Pressure GC (LPGC) column
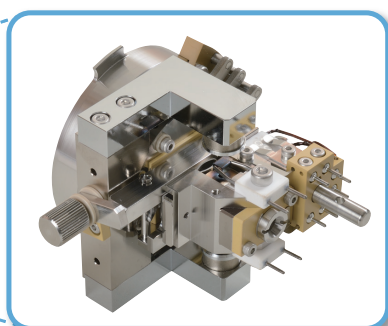
3. Turn the screw to release the stopper.
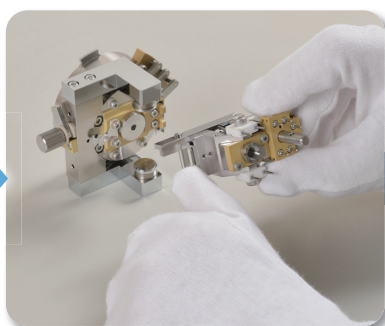
4. Remove the ion source.

5. Remove the chamber from the ion source and clean it.

Basic specifications and versatile hardware options for JMS-Q1600GC UltraQuad™ SQ-Zeta

The JMS-Q1600GC UltraQuad™ SQ-Zeta delivers all of the high performance capabilities required for GC-MS! Additionally, a wide variety of hardware options are available to support your application needs.
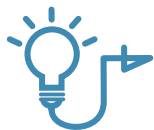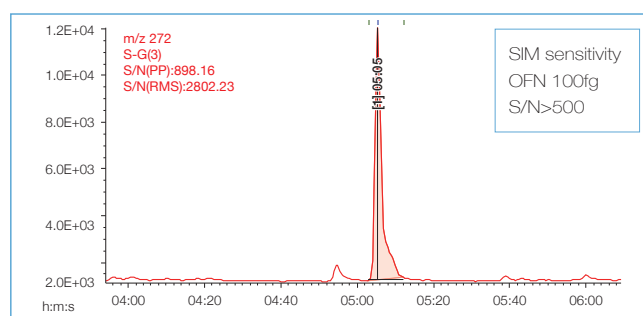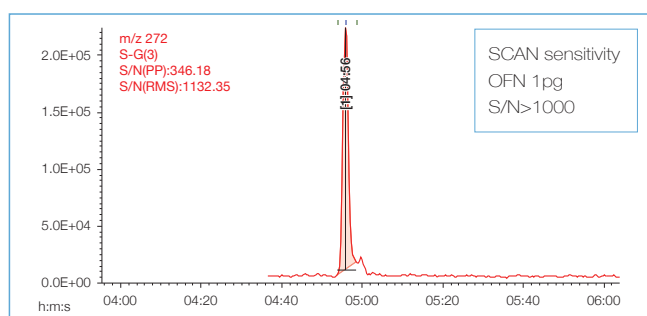
JEOL's unique high-precision hyperbolic-shaped quadrupole and Draw-In Lens achieve high sensitivity!

The JMS-Q1600GC UltraQuad™ SQ-Zeta is equipped with a multi-layered "Draw-in Lens" before the detector. This lens helps to reduce chemical noise and improve sensitivity by re-accelerating the ions. In addition, the Acquisition Processing Unit (APU) was upgraded to improve the efficiency and speed of data acquisition. With these state-of-the-art technologies, the JMS-Q1600GC UltraQuad™ SQ-Zeta is the most advanced GC-QMS system in the market with greatly improved detection sensitivity and SCAN speed.

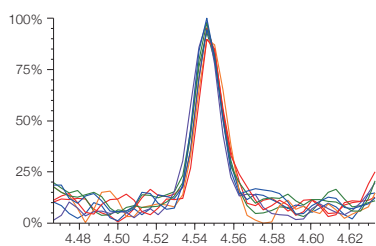## High sensitivity : SCAN OFN 1pg S/N>1000、SIM : OFN 100fg S/N>500

The standard EI ion source offers high sensitivity that is useful for quantitative trace analysis and qualitive analysis.

m/z 272
S-G(3)
S/N(PP):346.18
S/N(RMS):1132.35

SCAN sensitivity
OFN 1pg
S/N>1000

m/z 272
S-G(3)
S/N(PP):898.16
S/N(RMS):2802.23

SIM sensitivity
OFN 100fg
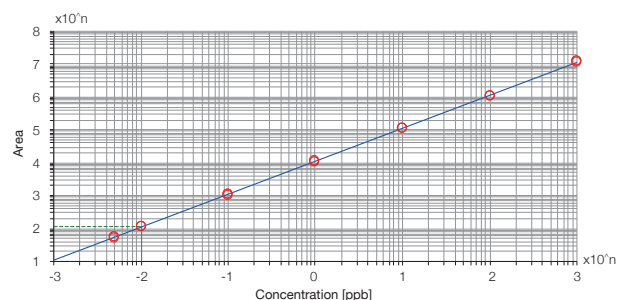S/N>500

OFN : Octafluoronaphthalene

IDL<5 fg

Eight sequential measurements of 20 fg of octafluoronaphthalene (OFN) were performed by using the standard EI ion source.
The instrument detection limit (IDL) is calculated based on the peak area and reproducibility of the extracted ion chromatogram for the molecular ion. An IDL of 2.6 fg was achieved for the system.
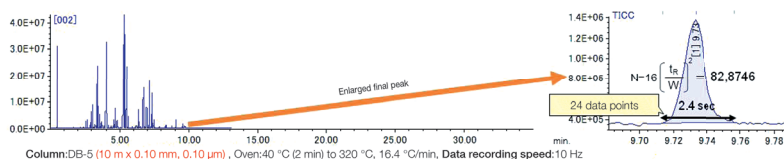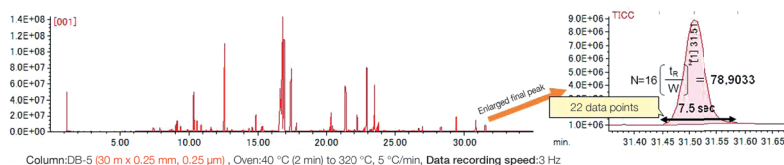
Wide dynamic range

OFN at concentrations ranging from 0.005 to 1,000 pg/uL were measured by using SIM mode with the standard EI ion source. A calibration curve with good linearity was obtained with a coefficient of determination of 0.999 or better. A wide dynamic range of more than 5 orders of magnitude is useful not only for quantitative analysis, but also for qualitative analysis of complex mixtures with different concentrations.

Injection No.	Peak Area
1	2,190
2	2,186
3	2,419
4	2,121
5	2,171
6	2,196
7	2,271
8	2,304

Response to Fast GC : Scan speed 22,222 u/sec

[001]
TICC
$N=16 \frac{t_R}{W} = 78.9033$
22 data points
7.5 sec
Column:DB-5 (30 m x 0.25 mm, 0.25 μm) , Oven:40 °C (2 min) to 320 °C, 5 °C/min, Data recording speed:3 Hz

[002]
TICC
$N=16 \frac{t_R}{W} = 82.8746$
24 data points
2.4 sec
Column:DB-5 (10 m x 0.10 mm, 0.10 μm) , Oven:40 °C (2 min) to 320 °C, 16.4 °C/min, Data recording speed:10 Hz

Enlarged final peak

Comparison of TICC of aroma oil using conventional GC condition and Fast GC condition
(Top: Conventional GC   Bottom: Fast GC)

Fast GC is a method that reduces measurement time while maintaining separation capability through the use of fast temperature ramps while using a short GC column with a narrow inner diameter. Because the chromatographic peak width becomes very narrow with Fast GC analysis, the mass spectrometer must have fast data acquisition capabilities.

The JMS-Q1600GC UltraQuad™ SQ-Zeta has a data acquisition and SCAN speed of 22,222 u/sec that is optimal for Fast GC analysis.

The left example shows the measurement results of 0.1 mL (neat) of commercially available aroma oil at a split of 100: 1 under conventional GC conditions and Fast GC conditions. Fast GC reduced the overall measurement to one-third of the analysis time.

Two unique EI ion sources
## Expanded analytical solutions!

The JMS-Q1600GC UltraQuad™ SQ-Zeta offers two types of optional EI ion sources. The Enhanced Performance Ion Source is a new high sensitivity ion source that enables ultra-trace analyses that were not possible before. The Dense Sample Analysis Ion Source allows the measurement of high concentration samples without dilution while minimizing source contamination.

Enhanced Performance Ion Source (EPIS, option) : IDL<1 fg

The EPIS offers the highest in-class sensitivity in the industry with an instrument detection limit of < 1 fg (OFN 5 fg, eight measurements). As a result, the EPIS offers a variety of benefits that include:

· Trace-level quantitative analysis
· Simplification of sample concentration analysis, reduction of sample introduction volume (contamination reduction)
· Replacement of quantitative measurement method from SIM to SCAN (simplification of measurement condition, non-target analysis possible).

The EPIS can be utilized not only for quantitative analysis but also qualitative analysis.
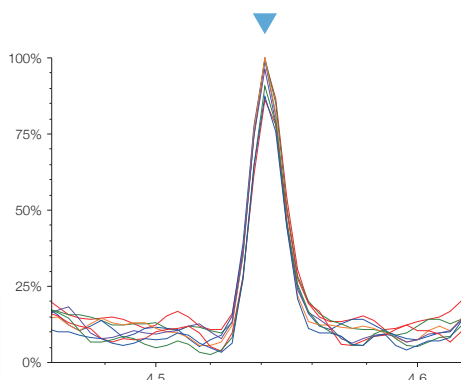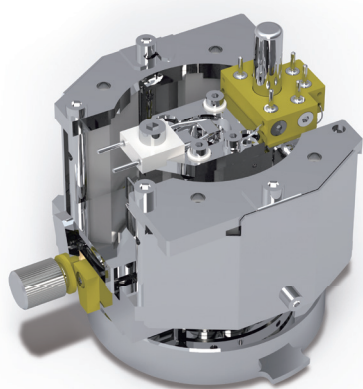
Injection No.	Peak Area
1	7,093
2	7,356
3	7,454
4	7,473
5	7,366
6	7,175
7	6,695
8	6,997

Eight sequential measurements of 5 fg of octafluoronaphthalene (OFN) were performed by using the EPIS ion source.
The instrument detection limit (IDL) is calculated based on the peak area and reproducibility of the extracted ion chromatogram for the molecular ion. An IDL of 0.6 fg was achieved for the system.

Dense Sample Analysis EI Ion Source (option) : SCAN OFN 1 pg S/N>20

The Dense Sample Analysis EI ion source is designed to reduce the contamination of the ion source and lens by enlarging the ion chamber opening. Additionally, this source has been optimized for measuring high concentration samples, such as volatile organic compounds (VOC) in waste solution, without dilution. This ion source is ideal for extending the dynamic range and linearity of the UltraQuad™ SQ-Zeta to high concentrations with high reproducibility and durability.
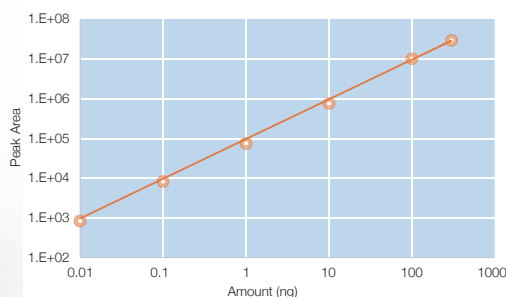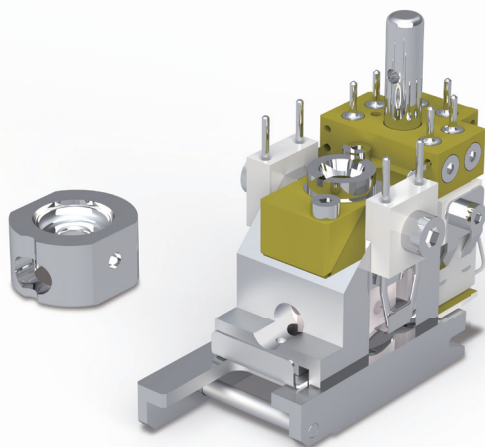
Amount (ng)	Peak Area
0.01	828
0.1	8,190
1	74,607
10	759,032
100	10,052,036
300	29,281,767
Correlation coefficient	0.9998

Linearity up to 300 ng was maintained for
p-Bromofluorobenzene used for VOC measurement.

Soft ionization with unique features
Widen your analysis capabilities!

With the JMS-Q1600GC UltraQuad™ SQ-Zeta, Photoionization (PI) and Chemical Ionization (CI) are available as soft ionization methods. Moreover, the standard EI ion source enables low-energy EI measurements which reduces the generation of fragment ions by decreasing the ionization voltage from 70 eV down to a range of 10-20 eV.

Soft ionization – useful for qualitative and quantitative analysis

EI is a hard ionization method that creates fragment ions and often results in minimal or no molecular ions.

On the UltraQuad™ SQ-Zeta, PI, CI, and Low-energy EI can be used as soft ionization methods to observe ions that provide molecular weight information, such as molecular ions and proton-adduct molecules.
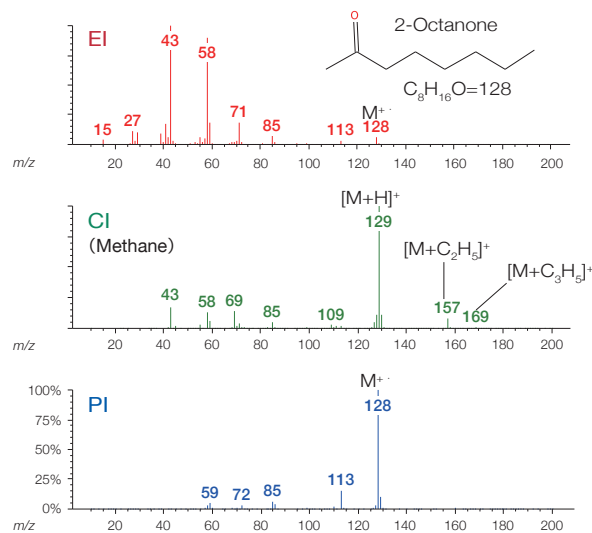
These soft ionization methods can be used for qualitative analysis to confirm library search results using the molecular ion information.
In addition, quantitative analysis using ions produced by them is also available.

Ionization energy: High
Hard ionization

Ionization energy: Low
Soft ionization

Mass spectra comparing ionization methods (Sample: 2-Octanone)

Photoionization EI/PI Combination Ion Source (option)

Photoionization (PI) is a soft ionization method that uses a vacuum ultraviolet (VUV) lamp. The EI/PI combination ion source allows both EI (Hard ionization) and PI (Soft ionization) without removing the ion source. All that is required for switching between EI and PI is to turn OFF the EI filament and turn ON the PI lamp or vice versa.
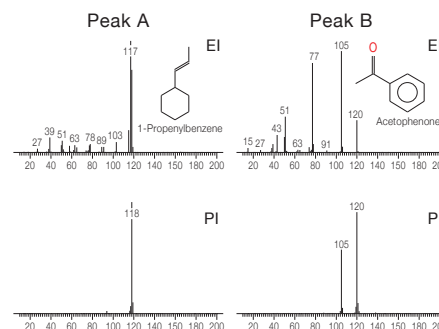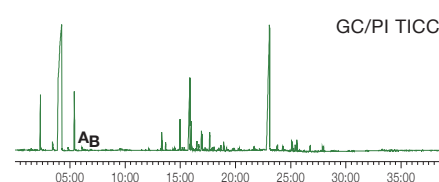
Features
▶ No need to replace the ion source
▶ No need to break vacuum
▶ No need for reagent gases
▶ Primarily for qualitative analysis
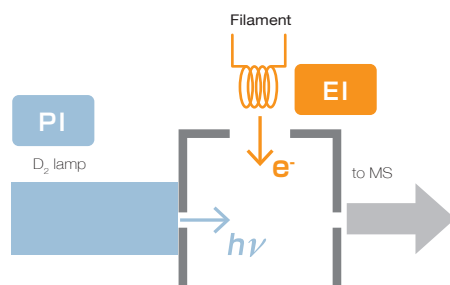
For PI; Lamp: ON, Filament: OFF
For EI; Lamp: OFF, Filament: ON

Schematic of EI/PI Combination Ion Source
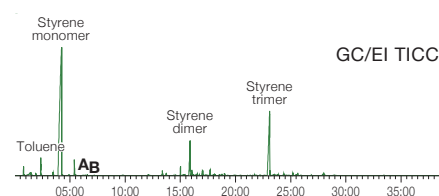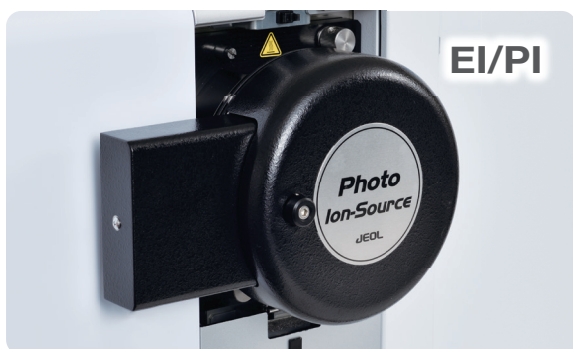
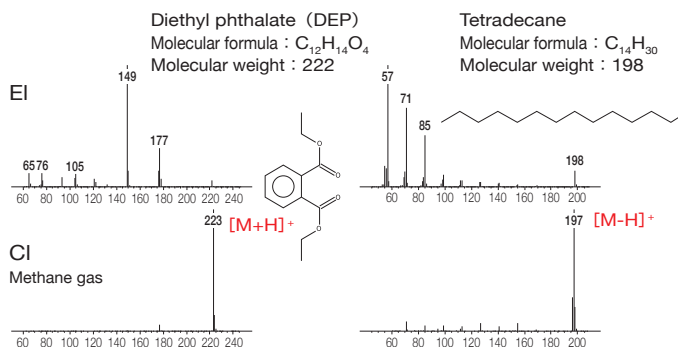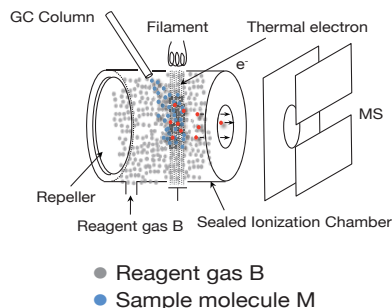Py/GC-MS measurement result of polystyrene foam

Aromatic hydrocarbons, which strongly absorb UV light, are preferentially ionized by PI, resulting in high sensitivity detection of their molecular ions.

Chemical ionization (CI) is a soft ionization method that produces molecular ion adducts through the reaction of sample molecules with a reagent gas in the ionization region. Methane, isobutane, and ammonia are typically used as the reagent gases.

Additionally, the CI method can be used for both positive- and negative-ion measurements. In general, positive-ion mode is used for qualitative analysis, such as confirmation of molecular weight, while negative-ion mode is commonly used for quantitative analysis of halogen-containing compounds, such as PCBs.

Features

▶ Need for reagent gas
▶ Positive-ion and negative-ion modes possible

Diethyl phthalate（DEP）
Molecular formula：$C_{12}H_{14}O_4$
Molecular weight：222

Tetradecane
Molecular formula：$C_{14}H_{30}$
Molecular weight：198

EI

CI
Methane gas

Ions obtained in positive mode

● Reagent gas B
● Sample molecule M

Positive mode：
● M + [B+H]⁺ → [M+H]⁺ + B （Proton adduct）
● M + [B+H]⁺ → [M+B+H]⁺ （Reagent gas adduct）
● M + [B+H]⁺ → [M-H]⁺ + [B+2H] （Hydride ion transfer）

Negative mode：
● M + e⁻ → [M]⁻ · （Resonance electron capture）
● M + e⁻ → [M-N]⁻ + N · （Dissociative electron capture）

Filament for Low Vacuum (option)

JEOL has developed a filament for low vacuum, which can perform stable EI measurements even when high amounts of oxygen are present.
This option makes it possible to perform TG measurements in an oxygen-rich atmosphere, in the same way as a synthesis process.
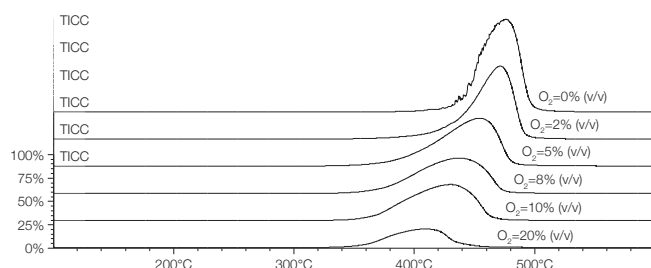
TICC of polystyrene after TG measurement at each oxygen concentration

For each TICC, a peak is generated by the decomposition of polystyrene. As the oxygen concentration increases, the starting temperature of gas generation becomes lower. These results indicate that the thermal decomposition temperature of polystyrene changes with oxygen concentration.

Direct MS Probes (option)

Direct MS probes are useful for measuring high-boiling-point components that are difficult or not possible to inject into a GC.
The JMS-Q1600GC UltraQuad™ SQ-Zeta offers two direct MS probe options.
Each probe is ideal for different types of samples in different physical states.

Direct Exposure Probe/F
(Direct Exposure Probe: DEP)

● Samples dissolved or dispersed in solvents are applied to a filament at the tip.
● Ideal for high boiling point compounds/thermally labile samples.

Direct Insertion Probe/C
(Direct Insertion Probe: DIP)

● Solid sample is put in a glass tube for measurement.
● Ideal for high boiling point compounds/samples that are difficult to dissolve in solvent.
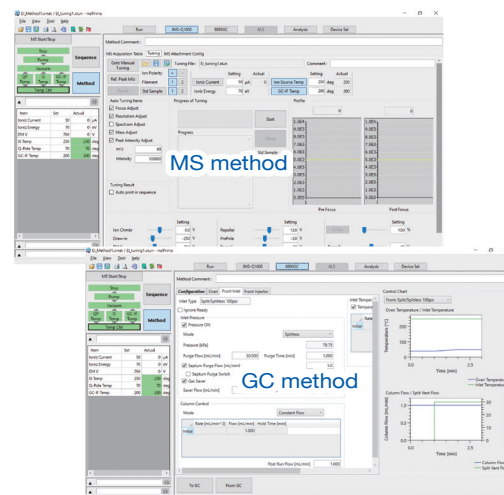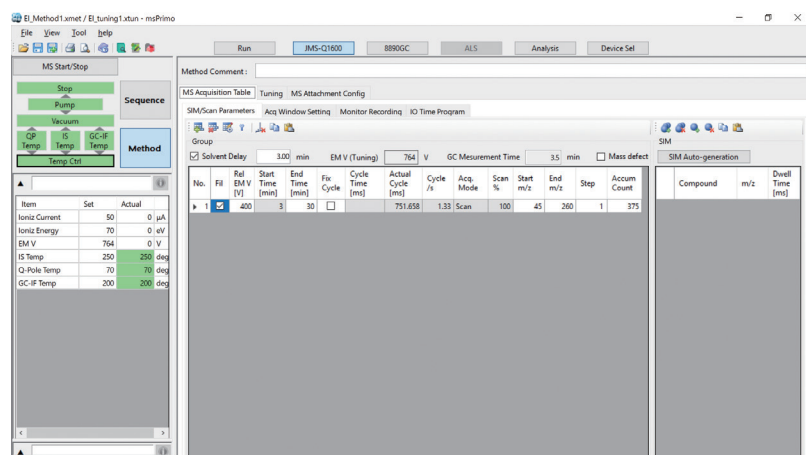
User interface designed for ease of use

MSPRIMO™ is the JEOL GC-QMS control software that was first released with the JMS-Q1500GC.
Functions that were previously divided into several windows in earlier software have been consolidated into a single window, making an intuitive and easy-to-use interface.

The status of each instrument parameter is always shown on the left side of the screen for easy confirmation of the instrument status. In addition, you can switch between tuning/calibration, GC method editing, MS method editing, and sequence setting within one window using a tabbed interface.

Capable of linkage among measurement, instrument control and analysis
Multi-function Sequence
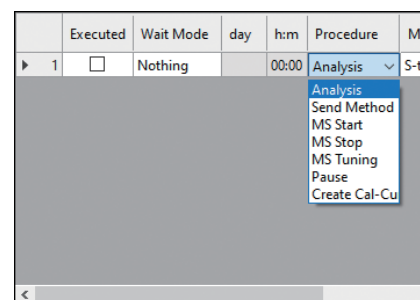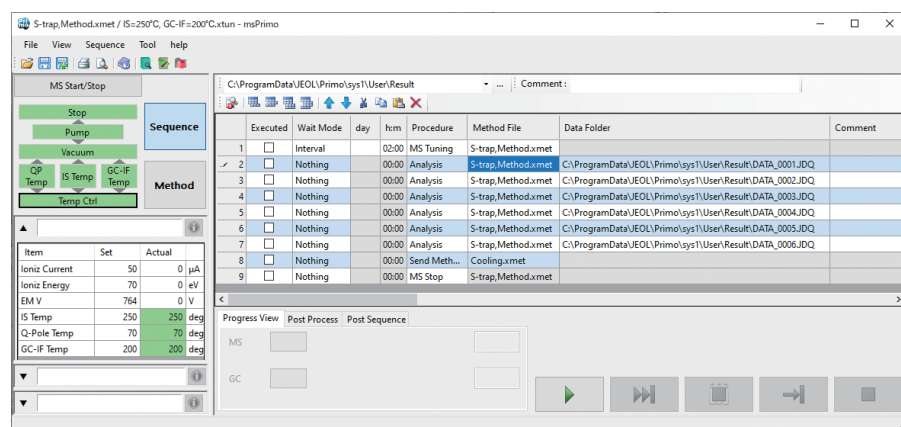
You can schedule not only the measurement (analysis) but also the start-up and shutdown of the instrument.

MSPRIMO™ features a multi-function sequence, allowing for measurement, instrument control, and analysis. Operation start time can also be set, making it possible to freely schedule all sequence items. This helps users manage their daily analytical operations, such as shutdown of the instrument after measurement, tuning at a desired position for sequential measurement, and quantitative analysis of the measured data.

Automatic SIM condition-creation function
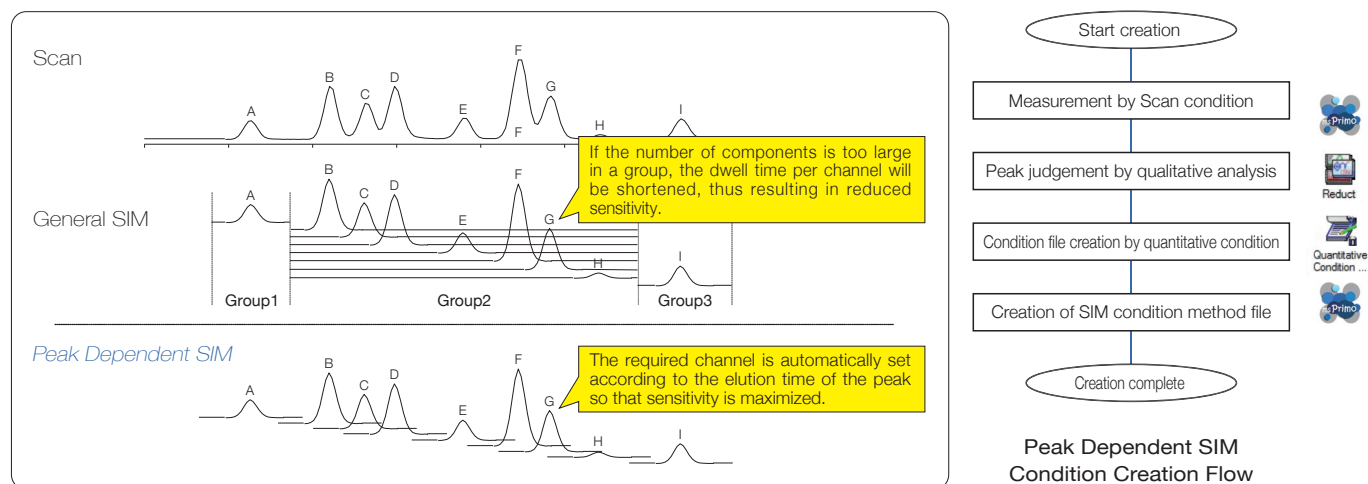## Peak Dependent SIM provides easy and high-sensitivity quantitative analysis

The new "Peak Dependent SIM" function simplifies the SIM grouping process by automatically optimizing these groupings based on analyte retention time in order to maximize sensitivity.
The maximum channel number for SIM measurements per 1 group is 100 channels, and the maximum group number is 500 groups.
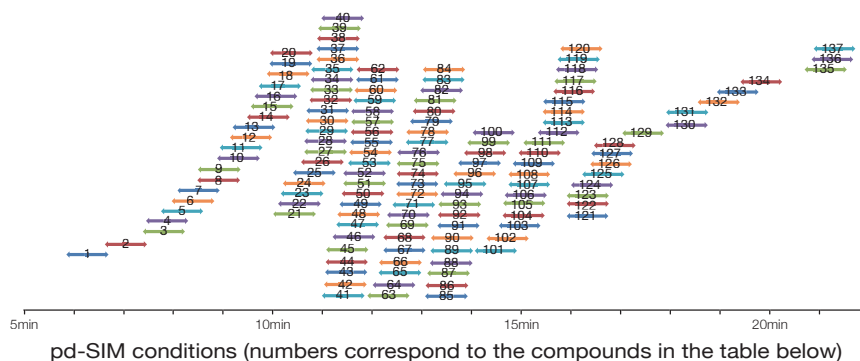

If the number of components is too large in a group, the dwell time per channel will be shortened, thus resulting in reduced sensitivity.

The required channel is automatically set according to the elution time of the peak so that sensitivity is maximized.

Peak Dependent SIM Condition Creation Flow

Start creation → Measurement by Scan condition → Peak judgement by qualitative analysis → Condition file creation by quantitative condition → Creation of SIM condition method file → Creation complete

Pesticide Analysis by Using Peak Dependent SIM (pd-SIM)

Study on the simultaneous analysis of regulated pesticides in drinking water

The figure on the right shows the pd-SIM parameters for all 134 pesticides that are targeted for the Japanese drinking water quality control regulations.
As shown, many components were observed to coelute in the 10-15 minute range. To handle this situation, pd-SIM used a SCAN measurement of the pesticides to automatically set the appropriate channel times for each Q-ion.

Additionally, setting these pd-SIM channels appropriately resulted in improved sensitivity over the traditional general SIM method mentioned previously.

Measurement results were stable for pd-SIM. The coefficient of variation for 5 ppb of pesticides (n=5) was less than 10%, indicating good reproducibility.

pd-SIM conditions (numbers correspond to the compounds in the table below)

#	Name	Q-ion (m/z)	R.T. (min)	C.V. (%)	r	#	Name	Q-ion (m/z)	R.T. (min)	C.V. (%)	r	#	Name	Q-ion (m/z)	R.T. (min)	C.V. (%)	r
1	Dichlorvos	185	6.14	1.0	0.999	47	Fenitrothion	277	11.61	6.4	0.998	93	Uniconazole p	234	13.69	2.9	0.997
2	Dichlobenil	171	6.92	1.0	0.999	48	Bromacil	205	11.63	2.5	0.998	94	Fenthion oxon sulfone	294	13.74	4.8	0.998
3	Etridiazole	211	7.68	1.4	0.999	49	(e)-dimethylvinphos	295	11.68	2.2	0.999	95	Buprofezin	105	13.80	1.8	0.999
4	Trichlorfon	79	7.76	—	0.989	50	Malathion	127	11.73	4.6	0.999	96	Isoxathion	105	14.00	1.8	0.998
5	Chloroneb	191	8.06	2.2	0.999	51	Chlorpyrifos oxon	270	11.76	4.4	0.996	97	Cyproconazole	222	14.09	1.7	0.998
6	Isoprocarb	121	8.28	3.1	0.998	52	Esprocarb	91	11.76	1.4	0.999	98	(z)-pyriminobac-methyl	302	14.21	3.4	0.999
7	Molinate	126	8.39	1.3	0.999	53	Quinoclamin	207	11.85	2.2	0.999	99	Fenthion sulfoxide	279	14.28	3.1	0.999
8	Fenobucarb	121	8.80	0.7	0.999	54	Metolachlor	162	11.87	1.8	0.999	100	Fenthion sulfone	310	14.36	2.7	0.999
9	Propoxur	110	8.81	1.4	0.999	55	Chlorpyrifos	197	11.89	2.6	0.999	101	Endosulfan β	195	14.40	3.7	0.999
10	Trifluralin	306	9.20	4.2	0.999	56	Cyanazine	225	11.91	5.5	0.999	102	Mepronil	119	14.64	1.3	0.998
11	Benfluralin	292	9.25	3.3	0.998	57	Thiobencarb	100	11.92	0.6	0.999	103	Chlornitrofen	317	14.88	5.3	0.998
12	Cadusafos	159	9.45	4.9	0.999	58	(z)-dimethylvinphos	295	11.92	2.5	0.998	104	Propiconazole-1	259	14.97	2.1	0.999
13	Pencycuron	125	9.51	2.2	0.999	59	Fenthion	278	11.95	1.8	0.999	105	Edifenphos	109	14.98	3.1	0.999
14	Dimethoate	125	9.80	5.6	0.998	60	Chlorthal-dimethyl	301	11.99	1.3	0.999	106	(e)-pyriminobac-methyl	302	15.01	2.1	0.999
15	Simazine	201	9.88	3.5	0.999	61	Isofenphos oxon	229	12.02	2.1	0.996	107	Propiconazole-2	259	15.08	1.9	0.999
16	Atrazine	200	9.95	3.2	0.999	62	Tetraconazole	336	12.03	1.6	0.999	108	Endosulfan sulfate	272	15.08	2.8	0.999
17	Diazinon oxon	137	10.03	2.3	0.997	63	Fthalide	243	12.24	3.2	0.999	109	Epn oxon	141	15.18	3.7	0.998
18	Cyanofos	243	10.20	1.4	0.999	64	Fosthiazate	195	12.35	5.4	0.997	110	Thenylchlor	127	15.29	1.3	0.999
19	Propyzamide	173	10.25	3.3	0.999	65	Pendimethalin	252	12.47	5.6	0.997	111	Tebuconazole	250	15.38	4.0	0.999
20	Diazinon	179	10.26	1.1	0.999	66	Cyprodinil	224	12.48	1.5	0.999	112	Pyributicarb	165	15.68	1.0	0.998
21	Pyroquilone	173	10.34	0.7	0.999	67	Dimethametryn	212	12.56	1.3	0.999	113	Iprodione	314	15.78	6.8	0.996
22	Chlorothalonil	266	10.43	2.7	0.999	68	Thiamethoxam	212	12.56	1.3	0.999	114	Pyridafenthion	340	15.78	1.6	0.998
23	Disulfoton	97	10.48	2.1	0.998	69	Isofenphos	213	12.63	3.4	0.999	115	Acetamiprid	152	15.79	7.2	0.999
24	Anthracene-d10	188	10.52			70	Methyl daimuron	107	12.75	10.8	0.999	116	Epn	157	15.99	3.9	0.998
25	Iprobenfos	91	10.73	2.0	0.998	71	Phenthoate	274	12.75	2.7	0.999	117	Piperophos	122	16.02	5.6	0.997
26	Tolclofos-methyl oxon.	249	10.90	1.8	0.999	72	Procymidone	283	12.83	0.9	0.999	118	Cumyluron	267	16.05	14.5	0.999
27	Fenitrothion oxon	244	10.96	6.4	0.998	73	Captan	79	12.83	1.8	0.998	119	Chrysene-d12	240	16.09		
28	Benfuresate	256	10.96	3.5	0.999	74	Triflumizole	278	12.84	5.3	0.998	120	Orysastrobin	205	16.14	5.4	0.997
29	Dichlofenthion	279	10.98	0.9	0.999	75	Butamifos oxon	244	12.85	5.8	0.998	121	Anilofos	226	16.26	3.1	0.999
30	Propanil	161	11.00	3.7	0.999	76	Dimepiperate	119	12.86	1.5	0.999	122	Bifenox	341	16.27	8.6	0.997
31	Terbucarb	205	11.01	2.0	0.999	77	Methidathion	145	13.02	3.4	0.998	123	Indanofan	174	16.27	5.7	0.999
32	Metribuzin	198	11.07	2.2	0.999	78	Propaphos	220	13.04	3.8	0.998	124	Furametpyr	157	16.36	1.4	0.999
33	Malaoxon	127	11.08	1.5	0.999	79	Tetrachlorvinphos	329	13.12	2.4	0.999	125	Phosalone	182	16.59	2.0	0.999
34	Chlorpyrifos-methyl	286	11.09	1.5	0.999	80	Butachlor	176	13.17	2.8	0.999	126	Pyriproxyfen	136	16.74	1.5	0.999
35	Bromobutide	119	11.10	2.7	0.999	81	Paclobutrazol	236	13.19	2.2	0.998	127	Cyhalofop-butyl	256	16.77	2.1	0.999
36	Alachlor	188	11.21	2.7	0.999	82	Butamifos	286	13.32	7.2	0.998	128	Mefenacet	192	16.82	3.0	0.998
37	Simeconazole	121	11.21	1.1	0.999	83	9-bromoanthracene	256	13.36			129	Pyraclofos	360	17.39	2.3	0.999
38	Tolclofos-methyl	265	11.23	1.4	0.999	84	Endosulfan α	195	13.37	6.7	0.999	130	Cafenstrole	100	18.28	2.4	0.998
39	Simetryn	213	11.25	1.2	0.999	85	Flutolanil	173	13.42	4.6	0.999	131	Etobenzanid	179	18.29	2.9	0.999
40	Ametrine	227	11.31	1.7	0.999	86	Napropamide	72	13.43	1.0	0.999	132	Boscalid	140	18.93	2.6	0.999
41	Metalaxyl	160	11.32	2.8	0.999	87	Metominostrobin	191	13.46	4.4	0.999	133	Etofenprox	163	19.32	3.2	0.999
42	Prometryn	241	11.36	4.8	0.999	88	Isoprothiolane	118	13.52	1.2	0.999	134	Thiacloprid	126	19.80	7.4	0.998
43	Cinmethylin	105	11.38	1.3	0.999	89	Isoxathion oxon	161	13.53	1.8	0.996	135	Difenoconazole-1	323	21.11	5.4	0.999
44	Mpp oxon	262	11.39	3.1	0.999	90	Pretilachlor	176	13.54	2.6	0.999	136	Difenoconazole-2	323	21.24	4.7	0.999
45	Dithiopyr	354	11.40	5.2	0.999	91	Thifluzamide	194	13.66	2.2	0.999	137	Pyrazoxyfen	105	21.28	1.9	0.999
46	Pirimiphos-methyl	290	11.54	1.9	0.998	92	Fenthion oxon sulfoxide	262	13.68	2.2	0.999						

Coefficient of variation for 5 ppb of 134 pesticide components

Proven Multi-Component Quantitative Analysis Software **"Escrime™"**

A full range of quantitative analysis functions to meet all your needs
Even qualitative analysis is possible.

Escrime™ is a multi-component quantitative analysis software package that can automatically calculate chromatogram peak areas, create calibration curves, and calculate quantitative values for target compounds. Additionally, this software allows the user to individually set or batch change the area calculation ranges and quantitative ions, which greatly reduces the time required for data processing.
The Escrime™ quantitative conditions and analysis parameters can be linked directly to the MSPRIMO™ instrument control software to simplify the overall quantitative analysis process.
The quantitative analysis report format can be customized according to the purpose and needs of the researcher.
Escrime™ is an essential tool for the quantitative analysis of multiple samples with multiple components.

Area Calculation Range

Example of Report Format
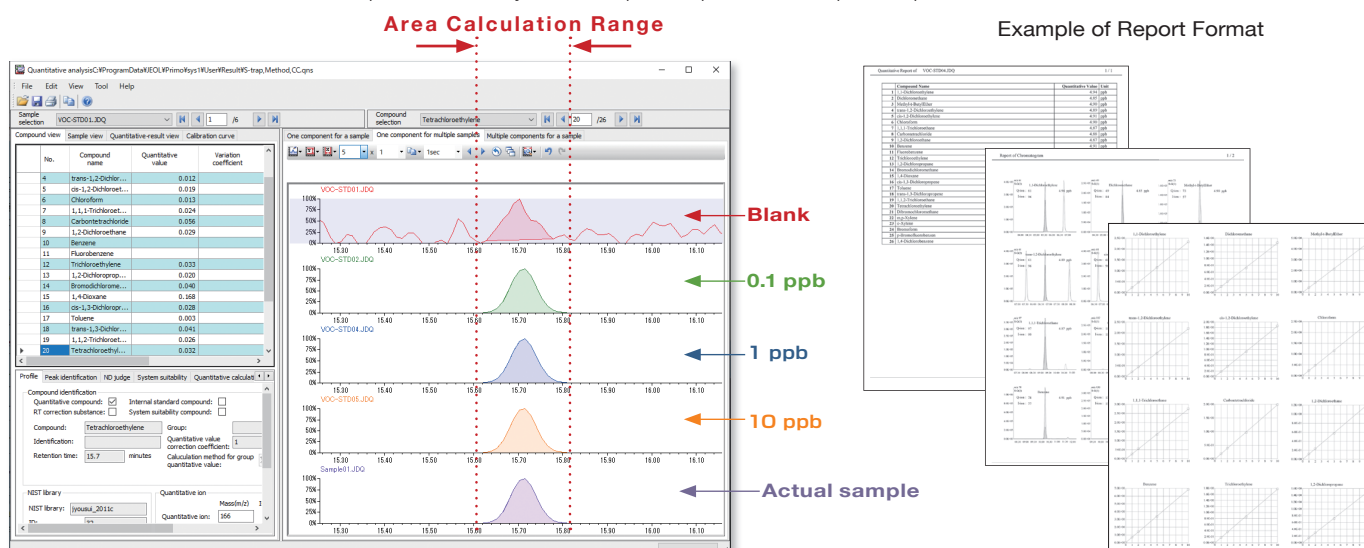
Component peaks in multiple samples or several component peaks in a single sample can be shown in the same screen.
In addition, peak area calculation range can be changed simultaneously, enabling bulk processing of multiple samples.

Escrime™ also features qualitative analysis capabilities that are available in a separate window. The qualitative analysis functions include automatic spectrum creation and library search, chromatogram peak list creation, and chromatogram creation.

Additionally, the qualitative analysis results can be copied and used for quantitative conditions by using drag-and-drop.
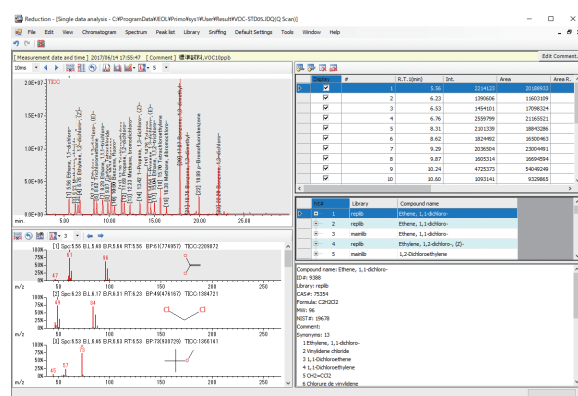
Software for Quantitative Analysis of Dioxins and PCBs **"TQ-Diok"**

TQ-Diok is quantitative analysis software specifically designed for dioxins and PCBs using benchtop GC-MS.
This software was developed by porting the features of DioK, a dedicated quantitative analysis software package for dioxins, into Escrime™.
TQ-Diok provides automatic quantitative analysis and reporting capabilities that greatly reduces the time required to analyze samples such as dioxins and PCBs.
This quantitative software combines the ease of use of Escrime™ with the expertise of Diok.
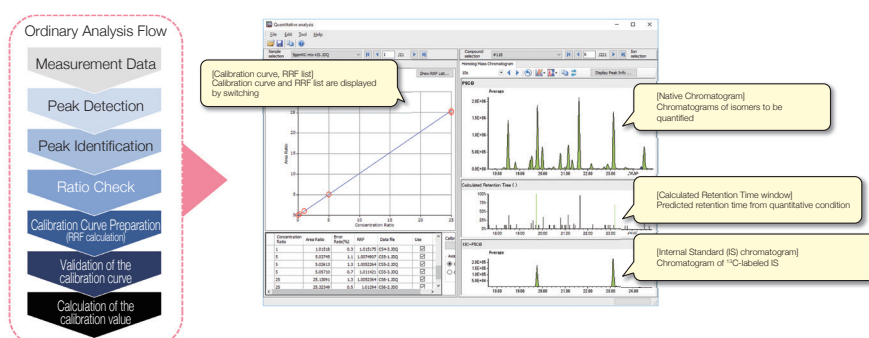
TQ-Diok simplifies and automates complicated analysis flow!
Anyone can easily perform quantitative analysis of dioxins and PCBs with this software.

Water analysis using a single GC column to measure VOCs, mold odor-causing substances, epichlorohydrin, styrene, and 1,2,3-trichlorobenzene

Headspace-GC/MS is commonly used for regulated water quality testing. However, in most cases, a column exchange between 2 different GC columns is required to test all targeted components.

In this study, we showed that the SQ-Zeta can be equipped with a single GC column (DB-1301, 60 m, 0.32 mm ID, 1 μm film thickness), to measure 2-methylisoborneol (2-MIB) and geosmin which are caused mold odor, volatile organic compounds (VOCs), as well as epichlorohydrin, styrene, and, 1,2,3-trichlorobenzene by only changing the instrument parameters.

The results showed good linearity for the calibration curves and good reproducibility at the limits of quantitation.
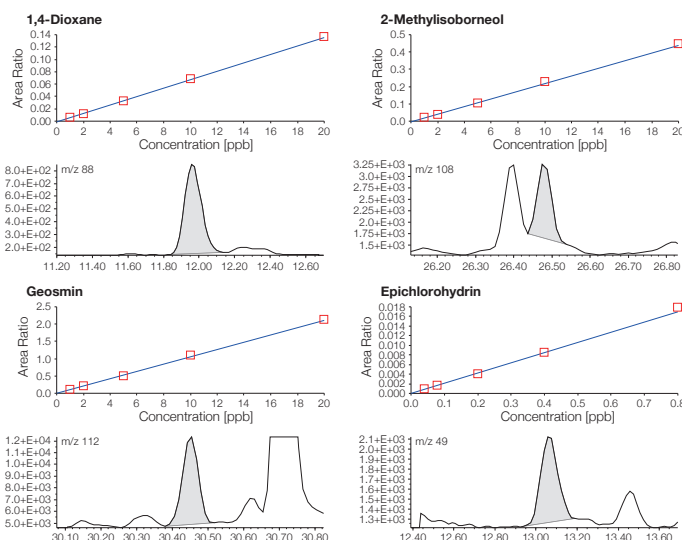
Extracted ion chromatograms and calibration curves of representative components

Compound Name	C.V. (%)	R	Compound Name	C.V. (%)	R	Compound Name	C.V. (%)	R
1,1-Dichloroethylene	0.7	0.9999	Trichloroethylene	0.1	0.9999	m-Xylene & p-Xylene	0.3	0.9992
Dichloromethane	1.1	0.9999	1,2-Dichloropropane	0.8	0.9999	o-Xylene	0.4	0.9999
t-Butyl Methyl Ether	0.4	0.9999	Bromodichloromethane	0.6	0.9999	Bromoform	0.6	0.9990
trans-1,2-Dichloroethylene	0.7	0.9999	1,4-Dioxane	1.1	0.9999	p-Dichlorobenzene	1.1	0.9999
cis-1,2-Dichloroethylene	0.6	0.9999	cis-1,3-Dichloropropene	1.7	0.9990	2-Methylisoborneol	4.5	0.9996
Chloroform	0.8	0.9999	Toluene	0.7	0.9999	Geosmin	3.4	0.9996
1,1,1-Trichloroethane	0.4	0.9999	trans-1,3-Trichloroethane	2.2	0.9985	Epichlorohydrin	2.6	0.9999
Carbon Tetrachloride	1.6	0.9999	1,1,2-Trichloroethane	3.0	0.9990	Styrene	1.5	0.9990
1,2-Dichloroethane	0.8	0.9998	Tetrachloroethylene	2.3	0.9996	1,2,3-Trichlorobenzene	9.0	0.9997
Benzene	1.2	0.9999	Dibromochloromethane	0.8	0.9991			

Coefficient of variation of relative standard deviation (n=5) and calibration curve at the limit of quantification for each component.

[limit of quantitation]
VOC (excluding 1,4-Dioxane): 0.1 ppb
1,4-Dioxane :1 ppb
2-MIB, Geosmin : 1 ppt
Epichlorohydrin: 0.04 ppb
Styrene, 1,2,3-Trichlorobenzene : 0.1 ppb

Analysis of low concentration PCBs in coating fragment

A sample solution was prepared by treating 5 g of a coating fragment in accordance with the "Measurement Methods for Low Concentration PCB-containing Wastes (5th Edition)" published by the Japanese Ministry of the Environment. A MBP-MPX PCB solution (Wellington Laboratories) was added as an internal standard to the sample solution just prior to sample analysis. The measurement conditions were based on the "Manual for Simple Determination of Trace PCBs in Insulating Oil (3rd Edition)" published by the Japanese Ministry of the Environment.

The results showed that the average relative response factor (AV-RRF) per cogener had good reproducibility with relative standard deviations (RSD) that ranged from 2.4% to 4.9%. The PCBs concentration in the coating fragment calculated by using the obtained Av-RRF resulted in 1.2 mg/kg.
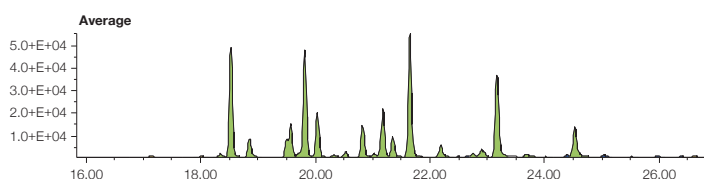
Average homologue chromatogram of PCBs in coating fragment

Standard Samples RRF List

No.	Type	Compound	Isomer	Av-RRF	SD	%RSD	OK
1	QNT	M1CB	#3	1.2646	0.0393	3.1	OK(10)
2	QNT	D2CB	#8	0.9534	0.0286	3.0	OK(10)
3	QNT	T3CB	#28	0.9436	0.0420	4.5	OK(10)
4	QNT	T4CB	#52	1.0958	0.0260	2.4	OK(10)
5	QNT	P5CB	#101	0.9984	0.0371	3.7	OK(10)
6	QNT	P5CB	#118	1.0185	0.0372	3.7	OK(10)
7	QNT	H6CB	#153	1.0146	0.0414	4.1	OK(10)
8	QNT	H6CB	#138	1.0684	0.0324	3.0	OK(10)
9	QNT	H7CB	#180	1.0343	0.0503	4.9	OK(10)
10	QNT	O8CB	#194	1.0675	0.0473	4.4	OK(10)
11	QNT	N9CB	#206	0.9905	0.0364	3.7	OK(10)
12	QNT	D10CB	#209	1.0616	0.0493	4.6	OK(10)

Reproducibility of average relative response factor

# Integrated qualitative analysis software **"msFineAnalysis iQ"**

Break free from qualitative analysis based on library search alone!
A higher level of qualitative analysis is possible by combining EI and soft ionization data!

Based on our highly acclaimed msFineAnalysis software for GC-TOFMS, the new msFineAnalysis iQ expands this integrated qualitative analysis capability into GC-QMS data analysis.

This software automatically combines the library search results from the EI data with molecular ion information from the soft ionization data, and then reports the results in a color coded table. This combination of EI and soft ionization results in improved accuracy for identifying unknowns when compared to relying on library database searches alone. Consequently, msFineAnalysis iQ is essential for the qualitative analysis GC-QMS data.
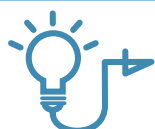
The risk of qualitative analysis by library search alone…
Are you sure that your identification is correct?

EI is widely used for GC-MS qualitative analysis due to the fact that EI library databases are widely available. However, because EI is a hard ionization method, it can often result in producing minimal to no molecular ion signal which can lead to mis-assignments for unknown compounds. In these cases, it is essential to use soft ionization to help with this situation.

As an example, the EI mass spectrum shown on the right had 5 candidates which were match factors (M.F.) of 800 or higher at the result of library search. Without additional information beyond this EI data, the compound identification would normally be the highest scoring candidate #1. However, when this compound is measured by using soft ionization, the molecular ion observed is m/z 314, which does not correspond to the molecular weight of candidate #1. As it turns out, candidate #2 has this molecular weight so this unknown compound is likely to be candidate #2.
Such misjudgment may occur when library search is used alone. This example shows that it is important to confirm the library search results by using soft ionization data.
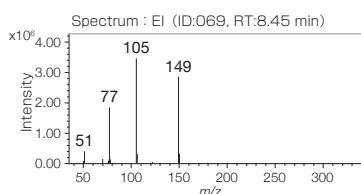
EI mass spectrum of Component A
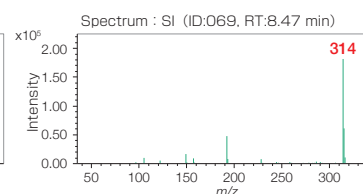
Soft ionization mass spectrum of Component A

#	Name of compound	M.F.	Molecular formula	Molecular weight
1	2,2'-(Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl) dibenzoate	828	C20 H22 O6	358
2	Diethylene glycol dibenzoate	821	C18 H18 O5	314
3	Benzoic acid, 2-(3-nitrophenyl)ethyl ester	810	C15 H13 N O4	271
4	1,3-Dioxolane, 2-(methoxymethyl)-2-phenyl-	802	C11 H14 O3	194
5	3,6,9,12-Tetraoxatetradecane-1,14-diyl dibenzoate	800	C24 H30 O8	446

Library search result for Component A: Top 5 Candidates

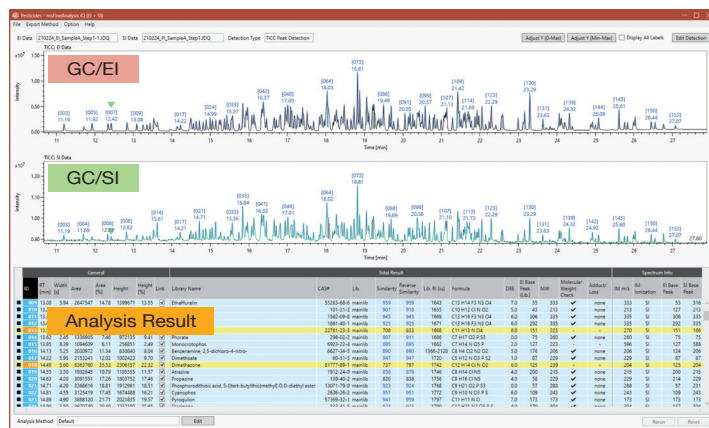**Library DB search and Analysis**   **Molecular ion search**
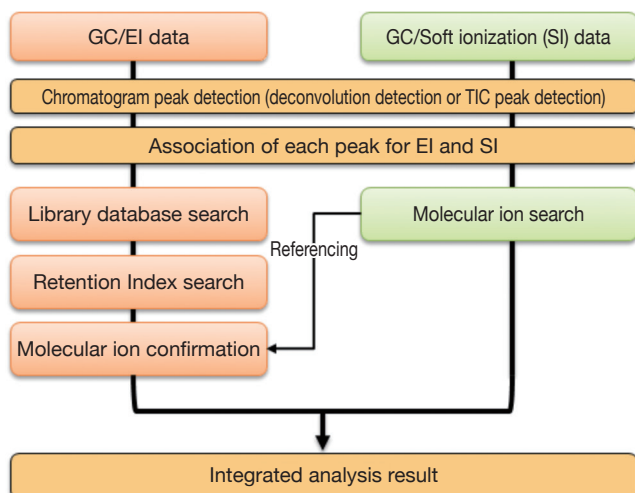
Work Flow of Integrated Analysis

msFineAnalysis iQ automatically performs the following steps.
① Peak detection (deconvolution peak or TIC peak detection)
② Link of EI and SI data (link)
③ Library search (EI)
④ Molecular ion search (SI)
⑤ Libray search result (EI, SI integration)
⑥ Integrated analysis result

Using EI and SI in combination with msFineAnalysis iQ provides a higher level of qualitative analysis results than relying on database searches alone.
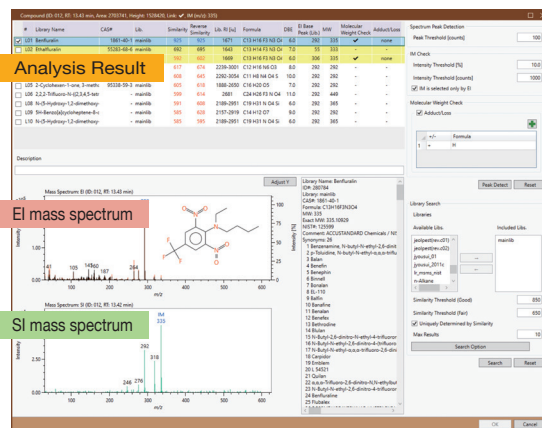
※ msFineAnalysis iQ is optional software

Integrated Analysis Result Window

Individual Analysis Window

The integrated analysis results screen show the overall analysis results which includes the EI/SI chromatogram data, chromatogram information, spectrum information, library search results, and molecular ion analysis results.

Double-clicking on a line in the analysis result list shows the individual mass spectrum analysis screen. In this screen, you can check and reanalyze the library search results and molecular ion analysis results.

Versatility of **msFineAnalysis iQ**

Deconvolution Peak Detection
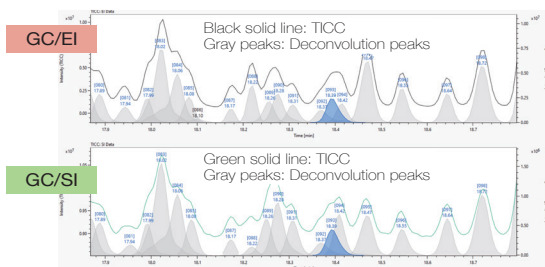
Deconvolution Peak Detection Example:
Each gray peak indicates a component detected by deconvolution.

With deconvolution peak detection, it is possible to detect low intensity peaks as well as coeluting peaks with varying intensities that cannot be easily confirmed in the TICC.

Single Analysis with Only EI Data
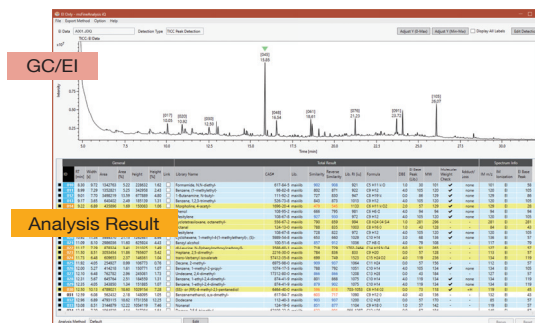
The software can also analyze GC/EI data alone when it is the only data available for your sample. In this case, the EI data is used for the molecular ion search, and this information is combined with the EI library search results.

Two-Sample Comparison (Differential Analysis)

Volcano Plot：
The volcano plot above represents the difference and reproducibility between two samples. This plot visually illustrates the characteristic components associated with each sample.

Another important feature of msFineAnalysis iQ is the variance components analysis function in which two similar samples can be directly compared in order to identify sample differences. This analysis function statistically compares two samples while also utilizing all of the normal msFineAnalysis iQ qualitative analysis capabilities described previously. Variance components analysis can be particularly useful for comparing complex materials that have subtle differences.

Qualitative Analysis Using Retention Index
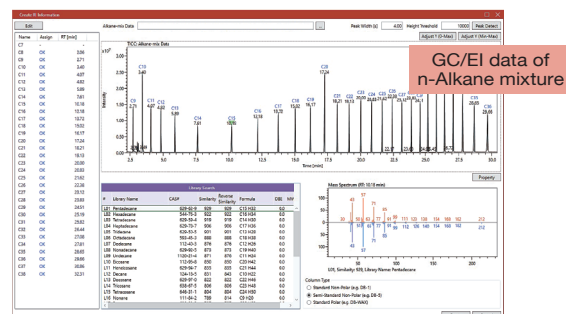
Retention Index Creation Screen

A retention index is a relative index value assigned to an analyte that is based on the retention times for an n-alkane standard mixture. This information basically allows the user to convert the target component retention time to a retention index value that can be directly compared to the retention index values available in the databases.

msFineAnalysis iQ can narrow down the search candidates by using the retention index value.

Pretreatment hardware options that meet your needs

Headspace Sampler of JEOL
MS-62071STRAP

■ Headspace GC-MS system

A headspace sampler is capable of sampling volatile compounds present above a solid or liquid sample and can be useful for applications involving VOCs in water, foods, and materials.

The headspace sampler developed by JEOL is a unique HS sampling system with 2 modes: loop mode and trap mode. Trap mode is particularly useful for high sensitivity measurements, such as mold odor-causing substances in water.

■ Multi-function Autosampler GC-MS System

The PAL System is a multi-function autosampler that can be customized to do liquid injections, automation for headspace sampling, solid phase microextraction (SPME), solid phase extraction (SPE), and liquid sample dispensing and dilution. Adding this to our GC-MS allows sequential pretreatment and GC-MS measurement.

The photo shows the system configuration in combination with the CTC multi-function autosampler (PAL RTC).
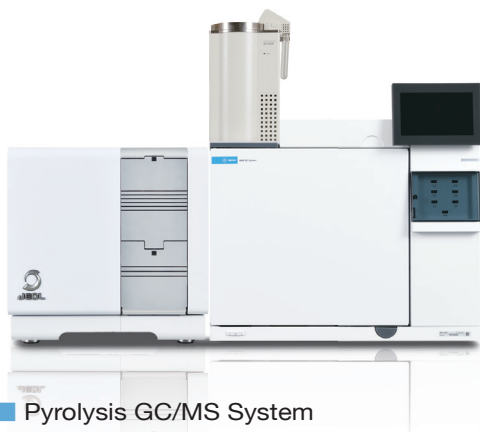
■ Pyrolysis GC/MS System

Pyrolysis GC-MS is an analytical technique that combines a pyrolyser with a GC/MS. This technique is very useful for the analysis of organic compounds generated from samples that are subjected to pyrolysis conditions. It can be used for the analysis of polymer materials such as synthetic polymers, rubbers, etc. The photo shows the system configuration with the Frontier Lab's Multi-Shot Pyrolyzer (EGA/PY-3030E) in combination with the Auto Shot Sampler (AS-1020E).

Sample : Sodium Formate HCOONa

Peak A: $2HCOONa \rightarrow H_2 + CO + Na_2CO_3$
$\qquad\qquad\qquad\quad H_2 + Na_2C_2O_4$
$\qquad\quad 2CO \rightarrow CO_2 + C$

Peak B: $Na_2C_2O_4 \rightarrow CO + Na_2CO_3$
$\qquad\quad 2CO \rightarrow CO_2 + C$
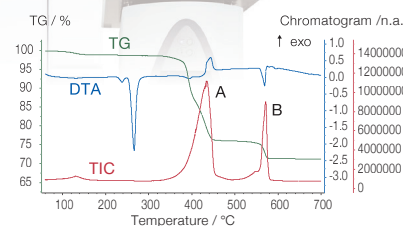
■ Thermogravimetry/Differential Thermal Analysis-MS System

For use in evaluating thermophysical properties, such as weight change and heat generation/absorption, associated with chemical change during the heating of a liquid or solid sample. When connected to an MS, the compounds generated during the heating process can be analyzed in real time. This system can be used for analysis of gases generated by heating materials, such as polymers.

JEOL Mass Spectrometer lineup

**Gas Chromatograph Triple Quadrupole Mass Spectrometer
JMS-TQ4000GC UltraQuad™ TQ**

Building upon the features of the JMS-Q1600GC, the UltraQuad™ TQ is a GC-MS/MS that uses JEOL's patented short collision cell technology to enable high throughput and high-sensitivity analysis of targeted, low-level analytes.
The ion accumulation and pulsed ion ejection capabilities of the short collision cell allow for highly-sensitive and -selective measurements even in high speed SRM mode (up to 1000 transitions/sec).
As a result of these strong capabilities, target applications for this system include the analysis of pesticides and other contaminants in environmental and food samples.

**High Performance Gas Chromatograph
– Time-of-Flight Mass Spectrometer
JMS-T2000GC AccuTOF™ GC-Alpha**

Our 6th generation gas chromatograph time-of-flight mass spectrometer has the highest resolution in its class at 30,000 and can determine compound composition from the accurate mass of measured ions. This system includes msFineAnalysis which simplifies the analysis of unknown compounds that are not registered in a library database.
As a GC-MS with strong qualitative analysis capabilities, it is used for a variety of applications, including material analysis and non-targeted analysis of environmental samples.

**High Resolution Mass Spectrometer
JMS-800D UltraFOCUS™**

The JMS-800D mass spectrometer is focused on the analysis of dioxins, PCBs, and other related trace environmental contaminants using HRGC/HRSIM modes.
This system has been equipped with a variety of capabilities to improve productivity and reduce maintenance costs.

**Matrix-Assisted Laser
Desorption/Ionization Time-of-
Flight Mass Spectrometer
JMS-S3000 SpiralTOF™-plus 2.0**

**Atmospheric Pressure Ionization High Resolution
Time-of-Flight Mass Spectrometer
JMS-T100LP AccuTOF™ LC-Express**

The JMS-S3000 has evolved into SpiralTOF™ -plus 2.0 with much wider dynamic range. The JMS-S3000 defines a new standard in MALDI-TOFMS performance and provides state-of-the-art analytical solutions for a wide range of research areas such as functional synthetic polymers, materials science, and biomolecules.

The AccuTOF™ LC-Express is the fourth generation of the successful AccuTOF™ LC series, a robust and easy-to-maintain, high-throughput mass spectrometer aiming for high productivity with multiple ionization methods.
JEOL's unique ionization technology, DART™ (Direct Analysis in Real Time) can rapidly provide accurate mass information. It is also easy to replace the ion source with the electrospray ionization (ESI) source for LC/MS operation, or with ColdSpray ionization (CSI) source.

Specifications

QMS Standard Configuration

Ion Source	Electron Ionization
	Ionization Energy 10 to 200 eV
	Chamber Temperature 100 to 300 ℃
Analyzer	High-precision hyperbolic quadrupole mass filter
	Plug-in prefilter system
Detector	Conversion dynode/ion multiplier detection
	Positive and negative ion detection
Evacuation System	Large differential evacuation system TMP 1 unit (Ion Source 200 L/s or equivalent, Analyzer 200 L/s or equivalent)
	Rotary Pump 1 unit (External)
Mass Range	1 to 1022 u
Resolution	2000 or better (FWHM, at m/z 614)
Scan Speed	22,222 u/s
Sensitivity (EI)	Instrument detection limit (IDL) 5 fg or less : Octafluoronaphtalene(OFN) m/z 272
	Scan S/N 1000 or more(RMS) : 1 pg Octafluoronaphtalene(OFN) m/z 272

Gas Chromatograph[MS-62111AGC]

Column Oven	Temperature range: Room temperature: + 4 to 450 ℃ (Minimum unit for temperature setting : 0.1 ℃ step)
	Effect of atmospheric temperature: Less than 0.01 ℃ per 1 ℃
	Heating program: Up to 20 stages settable (Maximum heating rate:120 ℃ /min)
Inlet	Split/Splitless inlet
	Maximum operating temperature: 400 ℃ (Extension up to 2 Ports possible)
Pressure Setting Range	0 to 680 kPa (For column of 0.200 mm or more diameter)
Total Flow	0 to 1250 mL/min (He)

Installation Layout Example of Standard Configuration

Unit（mm）
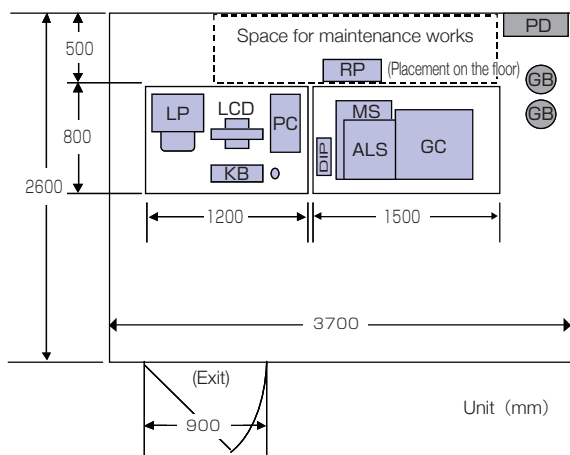
Symbol	Name
MS	QMS basic unit
GC	Gas Chromatograph
PC	PC
LCD	Display
KB	Keyboard
LP	Laser printer
RP	Rotary pump
PD	Power distribution panel
GC	Gas cylinder
DIP	PS for direct MS probe (optional)
ALS	GC Autosampler (optional)

JEOL Ltd.

3-1-2 Musashino Akishima Tokyo 196-8558 Japan   Sales Division Tel. +81-3-6262-3560   Fax. +81-3-6262-3577
www.jeol.com   ISO 9001 • ISO 14001 Certified

No.2208F023C(Bn)