Solutions for Innovation

JMS-T2000GC
AccuTOF™ GC-Alpha

Pursuing the ultimate in performance
and functionality

JEOL Ltd.

Alpha – The New Beginning

The Alpha takes you to a new world of mass spectrometry
Introducing JMS-T2000GC "AccuTOF™ GC-Alpha", the ultimate GC-MS with
superior performance and ease of operation

JMS-T2000GC AccuTOF™ GC-Alpha

2004

JMS-T100GC AccuTOF™ GC

· Mass resolving power ≥ 5,000
· Mass accuracy ≤ 5 ppm
· Spectrum recording speed up to 25 Hz
· Mass range up to *m/z* 2,000

2008

JMS-T100GCV AccuTOF™ GCv

· EI/FI/ED combination ion source
· Tuning assistant function
· Higher mass resolving power (5,000 → 6,000)

2012

JMS-T100GCV AccuTOF™ GCv 4G

· Higher mass resolving power (6,000 → 8,000)
· Better mass accuracy (5 ppm → 3 ppm)
· Faster spectrum recording speed (25 Hz → 50 Hz)
· Wider mass range (extended up to *m/z* 5,000)

2015

JMS-T200GC AccuTOF™ GCx

· EI/PI combination ion source
· msAxel software
· Higher mass resolving power (8,000 → 10,000)
· Better sensitivity (S/N 100 → 300)
· Wider mass range (extended up to *m/z* 6,000)

2018

JMS-T200GC AccuTOF™ GCx-plus

· msFineAnalysis software
· Automated mass calibrant inlet

JEOL developed orthogonal acceleration time-of-flight mass spectrometers (TOFMS) as our second type of high resolution MS after our successful conventional high resolution magnetic sector mass spectrometers. This new technology was initially released in 2001 as the JMS-T100LC AccuTOF™ in which atmospheric pressure ionization was implemented on this high resolution TOFMS for use with liquid chromatography (LC). This system was introduced into the global market at the Pittsburgh Conference in 2002 and was subsequently awarded the Pittcon Editors' Bronze Award in 2002 because it overcame the dynamic range limitations of other LC-TOFMS systems in the market, making it the first truly practical LC-TOFMS.

In 2004, a gas chromatograph (GC)-TOFMS version, the JMS-T100GC AccuTOF™ GC, was launched that was designed for use with vacuum ion sources that included EI, CI, FI, and FD. This system was the first GC-TOFMS to provide accurate mass measurements while achieving a mass resolving power of 5000 and a spectrum recording speed of 25Hz.

The legacy of the AccuTOF™ series continues to the AccuTOF™ GC-Alpha (and beyond).

Aiming for high performance while keeping it simple,

the **AccuTOF™ GC-Alpha** uses two new Key Technologies.
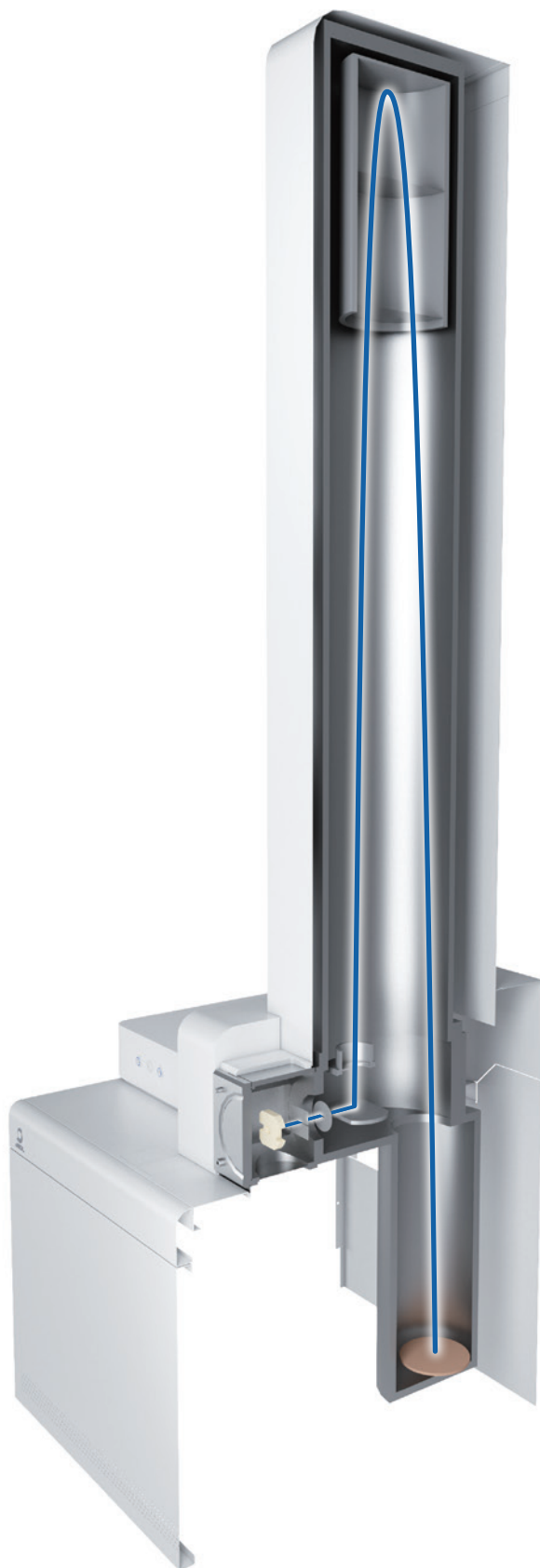
Key Technology 1

New high-performance hardware

The JMS-T2000GC AccuTOF™ GC-Alpha is the 6th generation JEOL GC-TOFMS and has an improved ion optics system to achieve ultra-high resolution.

The AccuTOF™ GC-Alpha is an orthogonal-acceleration time-of-flight mass spectrometer(oaTOFMS) with dual stage reflectron. It employs an ideal ion optical system realizing both high ion transmission(=sensitivity) and ultra-high resolution.

■ **Mass resolution and mass accuracy – Crucial for qualitative analysis**

$$R_{FWHM} = \frac{t}{2\Delta t}$$

R_{FWHM} : Resolving power

t : Ion time-of-flight

Δt : Ion peak width

The resolving power of a time-of-flight mass spectrometer is calculated according to the formula above. With this equation in mind, the new JMS-T2000GC AccuTOF™ GC-Alpha hardware was designed to achieve ultra-high resolution using the following principles:

▶ Make t longer: increase the flight distance 4 m

▶ Make Δt smaller: new ion optical system using dual stage reflectron

▶ Make Δt smaller: ion transfer system that can accommodate ions with a wide range of kinetic energy

With the newly developed hardware, the AccuTOF™ GC-Alpha features 6 times higher resolution than the first generation AccuTOF™ GC and has a mass accuracy of ≤ 1 ppm.

Acquiring unrivaled high-quality data, the AccuTOF™ GC-Alpha is the ultimate solution for GC-MS qualitative analysis.
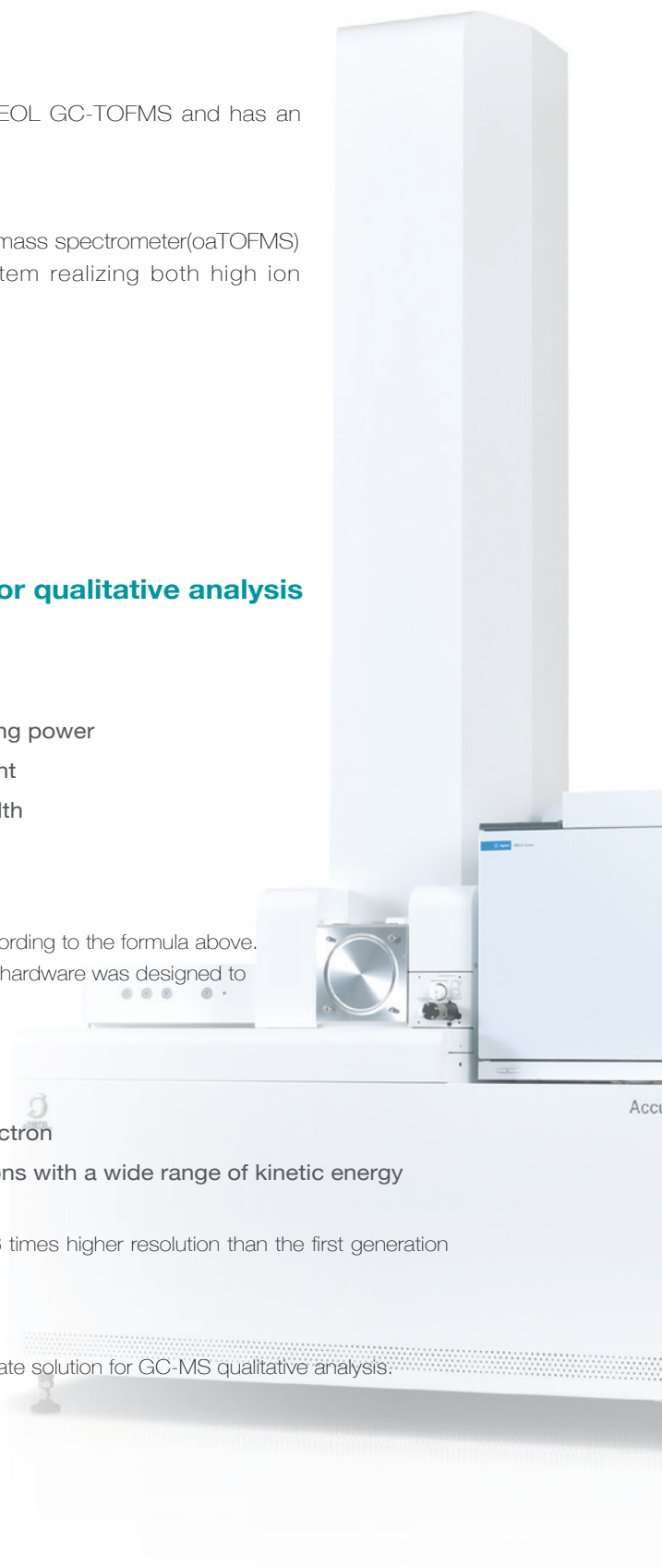
Basic Performance of AccuTOF™ GC-Alpha

High performance for both qualitative and quantitative analyses

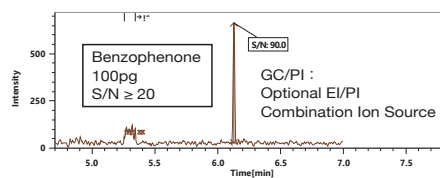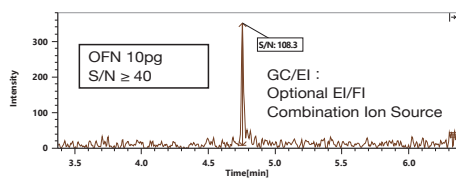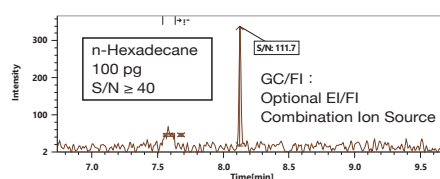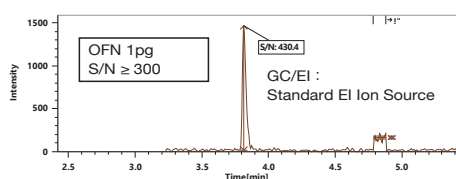Four **"High"** specifications and two **"Wide"** specifications achieved simultaneously

The JMS-T2000GC AccuTOF™ GC-Alpha is a high performance GC-MS system that simultaneously realizes high mass resolution, high mass accuracy, high sensitivity, high speed data acquisition, wide dynamic range, and wide mass range.

The high mass resolution and high mass accuracy offers unprecedented qualitative analysis results. The high-speed data acquisition can be used for advanced GC-MS measurements such as comprehensive two-dimensional GC (GCxGC), while the wide dynamic range is useful for not only quantitative analysis but also for qualitative analysis of complex mixtures. The wide mass range is especially useful for direct MS measurements, and high sensitivity enables unprecedented information about trace components.

The AccuTOF™ GC-Alpha is truly a high performance GC-MS system that removes the limitations for chemical analysis.
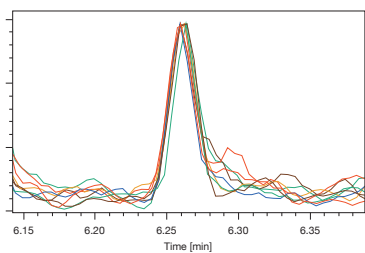
High Sensitivity

The standard EI ion source with ultra-high sensitivity is capable of micro volume trace quantitative analysis.

OFN 1pg
S/N ≥ 300
GC/EI :
Standard EI Ion Source
S/N: 430.4

n-Hexadecane
100 pg
S/N ≥ 40
GC/FI :
Optional EI/FI
Combination Ion Source
S/N: 111.7

OFN 10pg
S/N ≥ 40
GC/EI :
Optional EI/FI
Combination Ion Source
S/N: 108.3

Benzophenone
100pg
S/N ≥ 20
GC/PI :
Optional EI/PI
Combination Ion Source
S/N: 90.0

OFN: Octafluoronaphthalene

### Instrument Detection Limit: IDL=18.7 fg

Eight sequential measurements of 100 fg of octafluoronaphthalene (OFN) were obtained 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 18.7 fg was achieved for the system.

Injection No.	Peak Area
1	1187
2	1239
3	1126
4	1210
5	1236
6	1088
7	1044
8	1123
RSD(%)	6.2
IDL(fg)	18.7

Wide Dynamic Range: 4 orders

OFN at concentrations ranging from 0.1 to 1,000 pg/uL (4 orders) were measured using the standard EI ion source and a high degree of linearity was confirmed. The wide dynamic range is useful not only for quantitative analysis but also for qualitative analysis of complex mixtures with different concentrations.

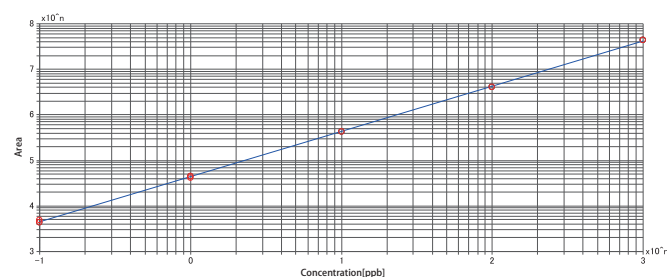### High Speed Data Acquisition:: 50 Hz

For GCxGC and Fast GC analyses, the chromatographic peaks are very narrow, thus requiring a mass spectrometer that supports high-speed data acquisition. The AccuTOF™ GC-Alpha is a good match for these advanced chromatographic techniques because it can acquire data at up to 50 spectra per second.
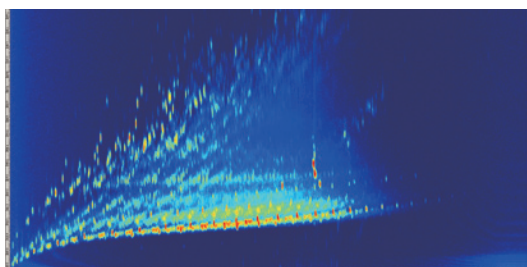
GCxGC/EI TICC of diesel fuel

Wide Mass Range: ~m/z 6,000

One of the features of time-of-flight mass spectrometers is their ability to measure a wide mass range. The upper limit of an ordinary GC-MS instrument is typically around m/z 1000, while the AccuTOF™ GC-Alpha can detect m/z 6000 and higher. This makes it possible to use direct probe MS methods such as field desorption (FD) to measure samples like oligomers.
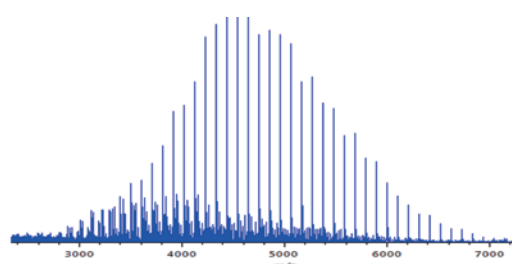

FD mass spectrum of polystyrene 5200

High Mass Resolving Power: 30,000

High mass resolving power is invaluable for qualitative analysis. Increasing the mass resolving power results in narrower mass spectral peaks, thus leading to the features below.

● Increased stability of the peak centroid = improved mass accuracy

MS: 0.1358–0.1891 / PFTBA-005 / EI+ / EI+ 2500V /   (245535)

CO 27.9943
N₂ 28.0055
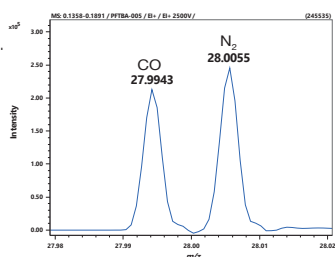
Mass separation of *m/z* 28
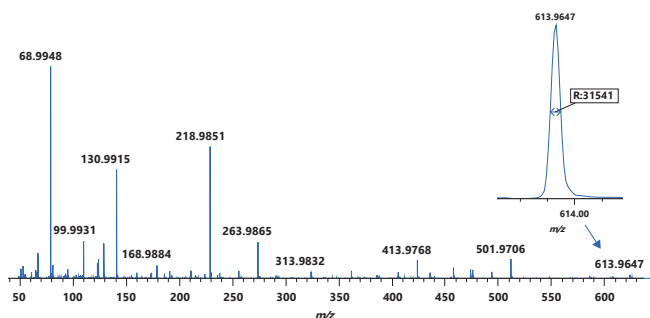
High Mass Accuracy: 1 ppm[*1]

* 1 Based on our standard for testing.

High mass accuracy makes it possible to determine the elemental compositions for the observed ions. Using the "drift compensation - multiple" mass calibration function, the average mass accuracy (absolute value) for 10 ions observed from methyl stearate was 0.05 mDa or 0.45 ppm.

Observation m/z	Composition formula	Calculation m/z	Error [mDa]	Error [ppm]
43.0542	$C_3 H_7$	43.0542	-0.06	-1.42
74.0363	$C_3 H_6 O_2$	74.0362	0.10	1.40
87.0440	$C_4 H_7 O_2$	87.0441	-0.01	-0.16
143.1067	$C_8 H_{15} O_2$	143.1067	0.03	0.22
185.1537	$C_{11} H_{21} O_2$	185.1536	0.05	0.26
199.1693	$C_{12} H_{23} O_2$	199.1693	0.04	0.19
213.1850	$C_{13} H_{25} O_2$	213.1849	0.08	0.39
255.2319	$C_{16} H_{31} O_2$	255.2319	0.03	0.11
267.2683	$C_{18} H_{35} O$	267.2682	0.05	0.18
298.2867	$C_{19} H_{38} O_2$	298.2866	0.06	0.20
Average mass accuracy (absolute value)			0.05	0.45

EI mass spectrum of PFTBA
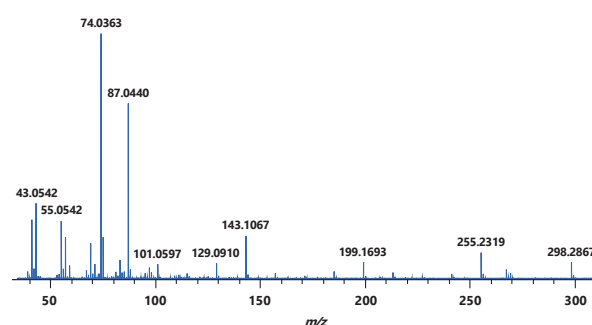
EI mass spectrum of methyl stearate

Benefits of
High Mass Resolving Power

When comparing the mass spectra of crude oil from the first generation AccuTOF™ GC and the latest JMS-T2000GC AccuTOF™ GC-Alpha, each ion is clearly separated and detected with the data obtained using the AccTOF™ GC-Alpha.

The difference in resolution is clearly evident in the KMD (Kendrick Mass Defect) plot for the FD mass spectrum of crude oil. The lower resolution of the first generation AccuTOF™ GC resulted in poor mass accuracy for unresolved peaks involving isobaric compounds at higher masses.

On the other hand, with the KMD plot drawn for the JMS-T2000GC AccuTOF™ GC-Alpha, peaks are separated and detected even at high mass, and good results are obtained even for components with high degrees of unsaturation (high KMD values).
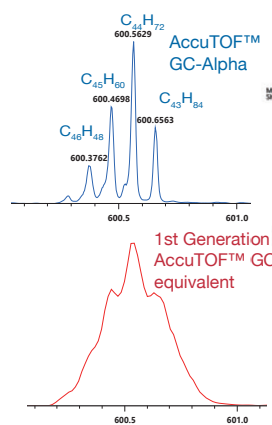
FD Mass Spectrum of Crude Oil

KMD Plot of Crude Oil

Left: AccuTOF™ GC-Alpha Data
Right: Data by 1st Generation AccuTOF™ GC equivalent

Benefits of
High Mass Accuracy

Higher mass accuracy means smaller mass error. With accurate mass analysis, it is common to consider the error and specify an "error tolerance" greater than the anticipated mass error. However, if the error tolerance is large, the number of candidate elemental compositions increases, thus making it difficult to judge which is the correct composition among multiple candidate elemental compositions.
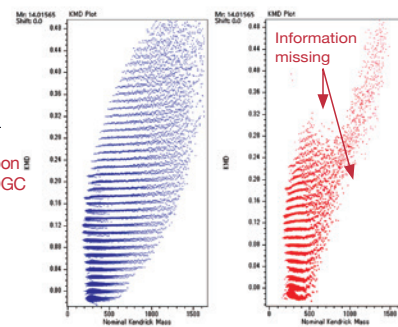
The higher mass accuracy of the AccuTOF™ GC-Alpha makes it possible to use a smaller mass tolerance which in turn reduces the number of candidate elemental compositions. As a result, the user can more easily determine the correct compositions!

Comparison of integrated analysis result of trilaurin

Error tolerance: 5 mDa

#	Elemental formula	DBE	Calculation m/z	Error [mDa]	EI Fragment Coverage
1	$C_{40} H_{70} N_4 O_2$	8.0	638.54933	0.07	100
2	$C_{39} H_{74} O_6$	3.0	638.54799	1.41	100
3	$C_{36} H_{66} N_{10}$	9.0	638.54664	2.76	100
4	$C_{29} H_{70} N_{10} O_5$	0.0	638.55252	-3.12	100
5	$C_{35} H_{70} N_6 O_4$	4.0	638.54531	4.09	100

Error tolerance: 2 mDa

#	Elemental formula	DBE	Calculation m/z	Error [mDa]	EI Fragment Coverage
1	$C_{39} H_{74} O_6$	3.0	638.54799	1.41	100
2	$C_{40} H_{70} N_4 O_2$	8.0	638.54933	0.07	85

With error tolerance of 5 mDa, 5 candidates have 100% EI fragment coverage.
With error tolerance of 2 mDa, only 1 candidate has 100% EI fragment coverage.

New Qualitative Analysis Capabilities offered by a Variety of Soft Ionizations

AccuTOF™ GC-Alpha provides multiple ionization methods
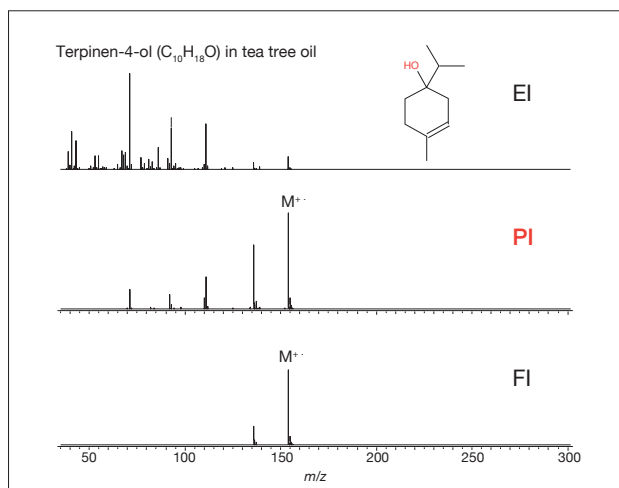
Soft ionization - a powerful tool for qualitative analysis

EI, the most widely used ionization technique in GC-MS, is superior in sensitivity and reproducibility and is supported by a variety of library searchable databases.

For any scientist using GC-MS in search of further information, what is ultimately important is molecular ion detection. EI, which uses a high ionization energy of 70 eV, generates numerous fragment ions, from which structural information is acquired. However, EI often fails to show strong molecular ion signals. Consequently, qualitative analysis results may be incorrect if they solely rely on database searches.

Thus, it is critical in GC-MS analysis to enhance the accuracy of qualitative analysis by using various soft ionization techniques in addition to EI. Chemical ionization (CI), photoionization (PI), and field ionization (FI) are all optionally available on the AccuTOF™ GC-Alpha. With the accurate mass measurement capability for all ionization techniques, elemental composition of the analyte can be reliably determined.

Terpinen-4-ol ($C_{10}H_{18}O$) in tea tree oil

EI

PI
$M^{+\cdot}$

FI
$M^{+\cdot}$

50   100   150   200   250   300
m/z

FI and FD ~ Ideal Soft Ionization Techniques for Molecular Weight Determination

FI and FD are extremely soft ionization techniques that provide lower internal energy to the analytes than EI and even CI, thus producing clear molecular ions.

As a result, FI and FD are ideal for molecular weight determination.

FI (Field Ionization)
▶ The sample is introduced to the ion source through GC or a standard sample inlet system.
▶ Unlike CI, FI uses no reagent gas; no need to choose a reagent gas appropriate for the analyte.

FD (Field Desorption)
▶ The sample is applied onto the emitter and directly introduced into the system.
▶ Suitable for analysis of thermally labile compounds.
▶ Ideal for samples soluble in nonpolar solvents.
▶ Analyzes powder samples dispersible in solvents.
▶ Analyzes low- to mid-polar metal complexes.
▶ Analyzes high molecular weight samples not supported in GC-MS, such as polymers.

Tip of the FD probe

Schematics of FI

Carbon Emitter

GC column

Anode (Emitter)

● Gas phase molecules (neutral)
● $M^{+\cdot}$, $[M+H]^+$, etc.

Cathode

e^-

MS

10kV

Schematics of FD

Carbon Emitter

Anode (Emitter)

● Condensed phase molecules (neutral)
● $M^{+\cdot}$, $[M+H]^+$, etc.

Cathode

Current

e^-

MS

10kV
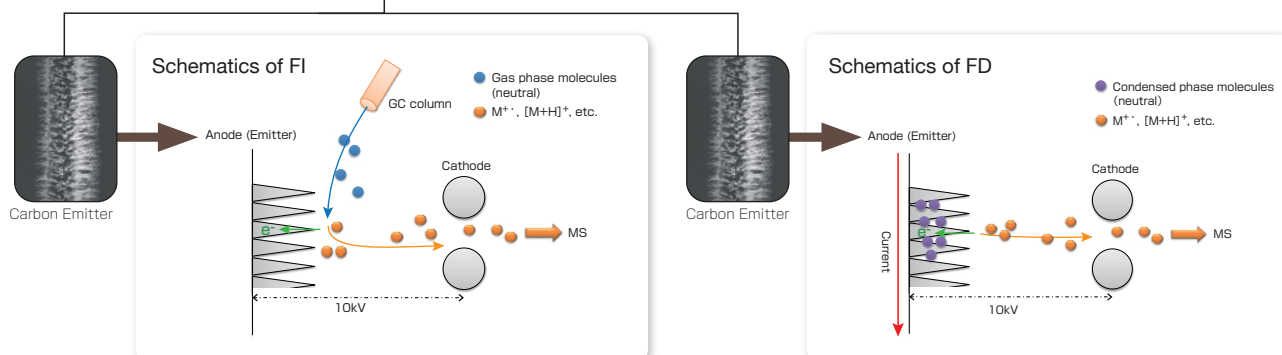
In FI and FD, ionization occurs by the removal of electrons from neutrals via the action of a high electric field.

FI and FD ~ EI/FI/FD Combination Ion Source (optional)
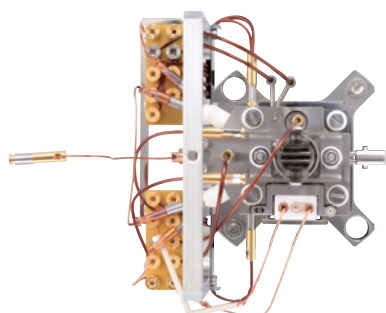
EI/FI/FD

A single ion source that supports both EI (hard ionization) and FI/FD (soft ionization) techniques.

Switching between EI and FI/FD is simple and quick.

Features
▶ No need to replace the ion source
▶ No need to break the vacuum
▶ No need for reagent gases

The following analyses are possible by using this combination ion source with GC:
▶ GC/EI for qualitative analysis through library search
▶ GC/FI for molecular weight determination
▶ Accurate mass measurement

PI (Photoionization) ~ EI/PI Combination Ion Source (optional)

EI/PI

PI is an ionization method that uses photons from a vacuum ultraviolet (VUV) lamp for ionization. The AccuTOF™ GC-Alpha has an optionally available combination ion source that offers both EI (hard ionization) and PI (soft ionization). This source makes it possible to switch between EI and PI by simply turning on/off the EI filament as well as the PI lamp.

Features
▶ No need to replace the ion source
▶ No need to break the vacuum
▶ No need for reagent gases

Filament

PI   EI

Deuterium Lamp   e⁻   To MS

hν

For PI; Lamp: ON, Filament: OFF
For EI; Lamp: OFF, Filament: ON

Schematics of EI/PI Combination Ion Source

Average mass spectra of diesel fuel   ● : n-Alkanes
● : Aromatic hydrocarbons

PI

FI

50   100   150   200   250   300   350   400
m/z

PI is particularly useful for the analysis of aromatic compounds in complex mixtures. These compounds produce high intensity peaks with PI because they strongly absorb UV light.

CI (Chemical Ionization) ~ CI Ion Source (optional)
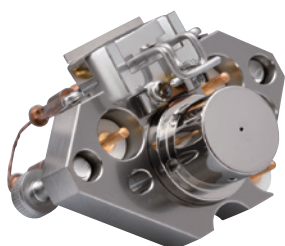
CI

CI is a classic soft ionization technique that is also optionally available with the AccuTOF™ GC-Alpha. The CI source comes equipped with three reagent gas inlet ports so that the user can easily switch the CI gas - typically methane, ammonia, and isobutane - using the instrument software. Customers that already use CI can choose this soft ionization option with confidence.

Aiming for high performance while keeping it simple,

the **AccuTOF™ GC-Alpha** uses two new Key Technologies.

Key Technology 2

A new generation of analysis software for simple, speedy operation

A new workflow has been devised to identify unknown compounds by GC-MS. In this workflow, the data analysis is performed by integrating the data obtained by hard ionization (EI) and the data obtained by soft ionization (FI, PI, CI) in order to identify the analytes present in a sample.(Patent pending)

Since its introduction in 2018, the msFineAnalysis software for the AccuTOF™ GC series has been well received as an innovative software solution for the automatic qualitative analysis of unknown compounds.

This software makes full use of the high-quality data obtained by the JMS-T2000GC AccuTOF™ GC-Alpha, thus providing a new approach to qualitative analysis for identification of unknown compounds.

■ Evolution into Version 3

Version 3 of msFineAnalysis streamlines the software operation and adds a new function in which 2 similar samples can be directly compared for differential analysis. This new, enhanced version of msFineAnalysis allows the operator to easily accomplish qualitative analysis of unknown compounds as well as for compounds that are unregistered in the EI mass spectral libraries.

Features of msFineAnalysis

▶ Combines EI/SI data for automatic qualitative analysis
▶ Chromatographic peak deconvolution
▶ Group analysis for extracting compounds with common substructures
▶ Differential analysis for directly comparing 2 samples
▶ Also supports the analysis of EI data alone

msFineAnalysis provides quick and efficient data analysis so that the user can spend less time analyzing data and more time on research and creativity!

Integrated Analysis using msFineAnalysis

Auto non-target analysis combining data acquired by GC/EI and GC/soft ionization

msFineAnalysis guarantees **shorter** working time, **improved** work efficiency, **enhanced** quality analysis results.

The msFineAnalysis software provides qualitative results by combining data acquired by EI ionization and soft ionization (FI, CI, or PI) in a simple, speedy manner.

The software supports two different component detection process -- TICC peak detection and deconvolution detection -- to separate overlapping chromatographic peaks by using accurate mass information. msFineAnalysis Version 3 provides a new function for finding differences in samples. This function displays a comparison of two samples (such as a normal product and abnormal product) and provides an analysis with integrated interpretation.

msFineAnalysis continues to satisfy your most demanding needs for qualitative analysis.

Integrated Analysis Workflow: Fully Automated Qualitative Analysis

The software automatically identifies the molecular ions for all components detected, and calculates molecular and fragment ion elemental compositions. This software also automatically performs qualitative analysis for any components that are not registered in the EI mass spectral libraries.

Library Search and Analysis

- GC/EI data
- Chromatogram peak detection
- Link of each peak of EI, SI
- 1. Library search
- Molecular ion confirmation in EI/SI mass spectra

Molecular Ion Search and Analysis

- GC/Soft Ionization (SI) data
- 2. Molecular ion search
- 3. Accurate mass analysis for molecular ion
- 4. Isotope pattern matching analysis

Reference, Extension

5. Accurate mass analysis for EI fragment ions with the elemental composition of (1) and (3)

Integrate qualitative analysis results

msFineAnalysis also supports analysis of GC/EI data alone. If you only have EI data due to a lack of time or limited amount of sample, you can still use the software! msFineAnalysis can offer better quality search results based on the library search with additional accurate mass analysis.

Introduction of auto-analysis function using msFineAnalysis

~ auto-qualitative analysis that

1.NIST Library Search

Degree of Similarity:Poor

EI mass spectrum observed

Degree of Similarity:Good

Degree of Similarity:Poor

NIST Library Search

Performs a library search first to identify the unknown compounds in the EI mass spectrum according to the degree of similarity.

2. Molecular Ion Search

EI

FI

$M^{+ \cdot} = 326.188$

Searches for a molecular ion; uses the molecular ion found here for the subsequent analysis. Can also select the molecular ion in the EI mass spectrum.

3.Accurate Mass Analy

Integer Mass: 326

Num

C_8

$C_{16} H_{26} N_2$

$C_{21} H_{26}$

$C_{12} H_{28} N_3 O_7$

$C_{10} H_{26} N_6$

Exact Mass: 326.188

Narr

C_{21}

Performs exact mass ion to filter the molec

Intuitive GUI

A single view shows the GC/EI and GC/SI chromatogram data, chromatogram information, library search results, and accurate mass analysis results.

GC/EI data
Black solid line: TICC
Gray peaks:
Deconvolution peaks

GC/SI data
Green solid line : TICC
Gray peaks:
Deconvolution peaks

Chromatogram molecular ion information

Qualitative analysis result

Library search result
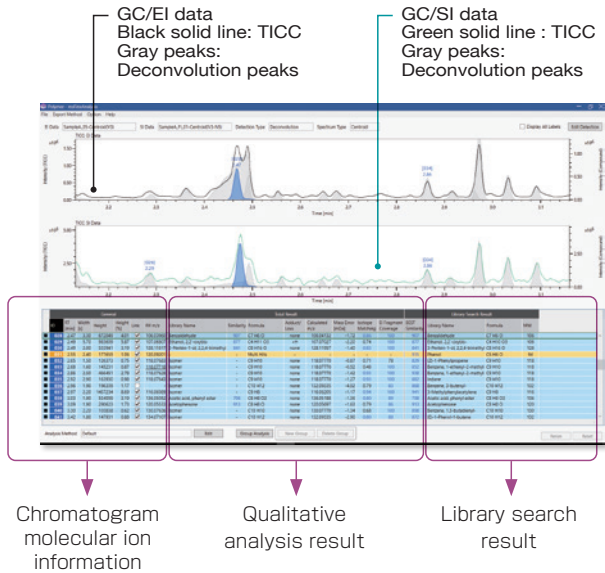
Group Analysis

Group analysis extracts the analytical results for components that share a common ion (molecular ion/fragment ion) or neutral loss. Specifying a fragment ion or neutral loss is effective for the analysis of components sharing a similar partial structure, such as congeners. Specifying a molecular ion enables analysis of isomers. Group analysis can extract results for up to 5 groups at a time.

Extracting components containing a specified ion or neutral loss

Specifying an observed ion or neutral loss

The operator can review analytical results of certain compound groups quickly by using, for example, C_6H_5 fragment ions specific to aromatic compounds or Cl neutral losses to indicate the presence of chlorinated compounds.

Two-Sample Comparison (Differential Analysis)

Integrated analysis result

Volcano Plot

Classification

Differential analysis result
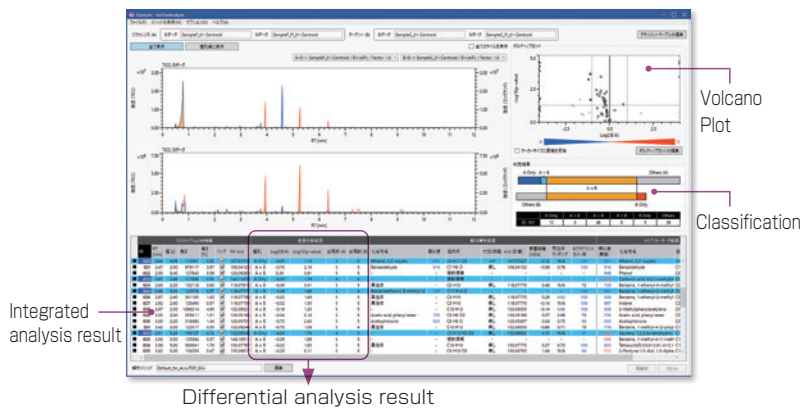
The 2-sample comparison function provides Volcano Plots where the Y axis represents the statistic reproducibility using p value, and the X axis represents the intensity ratio between the 2 samples. These plots can visually illustrate the distinguishing components between the two samples.

After determining whether there are differences, integrated analysis is performed for all components.

For the 2-sample comparison, values of n=1, 3, 5 are possible for the number of measurements for each sample. For the case of n=1, the result will be a simple comparison of intensity without consideration of statistical reproducibility. This function can be utilized even when it is difficult to obtain more than one measurement for each sample.

~ combines 5 qualitative techniques for the peaks detected ~

...sis of Molecular Ions

...erous formula candidates

$C_{24}N_9O_5$ $C_{17}H_{22}N_6O$
...O$_5$ $C_{15}H_{20}N_9$
...O$_3$ $C_{24}H_{24}N$
$C_{11}H_{22}N_{10}O_2$
...O$_6$ $C_{19}H_{24}N_3O_2$
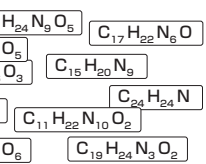
...ow down the candidates!

$...H_{26}O_3$

...analysis on the molecular ...ular formula candidates.

4. Isotopic Pattern Analysis

Isotopic patterns of molecular ions observed

Pattern Analysis

Formula Candidates
$C_nH_mO_l$ $C_xH_yO_z$
$C_aH_bO_c$

Formula Candidate 1): $C_aH_bO_c$
Degree of Similarity: Poor

Formula Candidate 2): $C_nH_mO_l$
Degree of Similarity: Good

Formula Candidate 3): $C_xH_yO_z$
Degree of Similarity: Poor

Multiple formula candidates often appear during molecular ion exact mass analysis. When this happens, isotopic pattern analysis is effective for filtering the formula candidates.

5. EI Fragment Ion Accurate Analysis Result

Formula Candidate 1): $C_aH_bO_c$

EI When the chemical formulas for the fragment ions were calculated using the elements present in $C_aH_bO_c$, three ions failed to produce a formula.

Formula Candidate 1):
$C_aH_bO_c$ - False

Formula Candidate 2): C_nH_mN

EI When the chemical formulas for the fragment ions were calculated using the elements present in C_nH_mN, all ions produced a formula.

Formula Candidate 2):
C_nH_mN - Correct

Molecular ion formula candidates can be filtered by the fraction of successful fragment formula calculations. The results of fragment formula calculations contain partial structural information, which can be used to determine the structural formula.

Integrated Analysis Applications using msFineAnalysis

msFineAnalysis automatically performs qualitative analysis for all detected components, regardless of whether those compounds are present in a database. Molecular formulas (molecular ion, protonated molecule, etc.) are obtained from the soft ionization data, while the structural information (fragment ions) is obtained from the EI data automatically. This offers an integrated analysis that is more specific and informative than conventional GC-MS analysis, which depend solely on library database searches.

Integrated Analysis of an Acrylic Resin by Py/GC-TOFMS (MSTips No.300)

Interpreting **Pyrolysis GC-MS**

By measuring a polymer sample or a material sample by Py/GC-MS, information including the presence of additives, polymer structure, and polymerization process can be obtained from the analysis. These components are often not registered in the library and not determined by conventional GC-MS.

For components that are not registered in a library database, the msFineAnalysis integrated analysis functions can be very useful.

msFineAnalysis supports the analysis of polymer and material samples which was not previously possible.
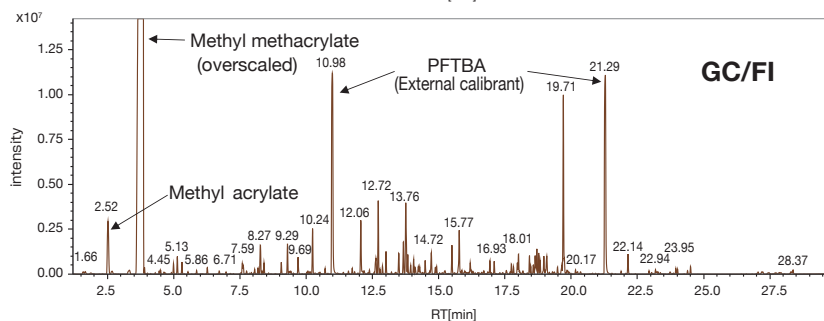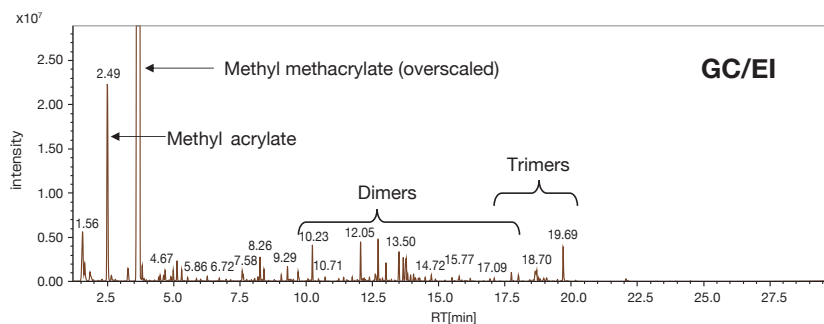
TIC Chromatogram of Acrylic Resin
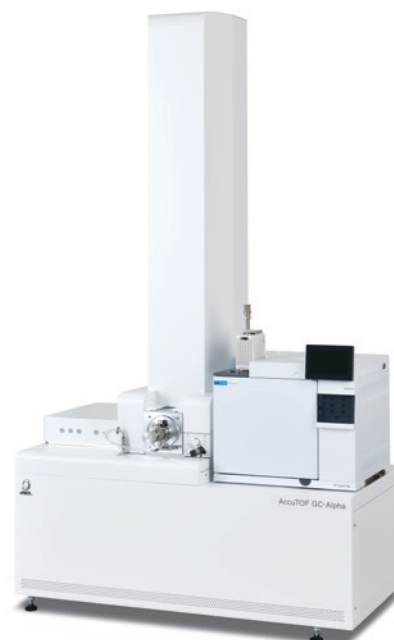
Installation example of a pyrolyzer

Comparison of qualitative analysis results :
Left: Integrated Analysis by msFineAnalysis, Right: Library Database Search
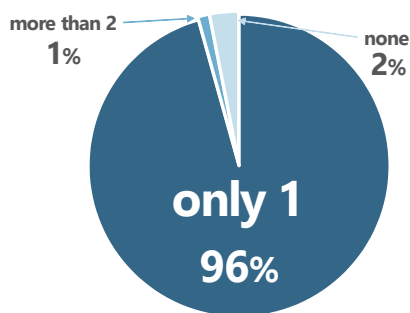
[Integrated Analysis by msFineAnalysis]
Classified by the number of molecular formula candidates
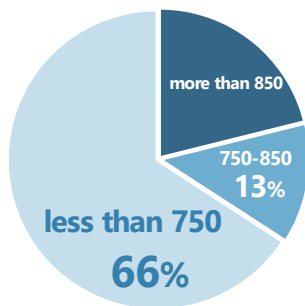
[Qualitative Analysis by Library DB Search Only]
Classified by the Match Factor Score

[Integrated Analysis by msFineAnalysis]
- One Molecular Formula Candidate : 154 components (96%)
- More than One Molecular Formula Candidate : 2 components (1%)
- No Molecular Formula Candidate : 5 components (2%)

[Qualitative Analysis by Library DB Search Only]
- Score 850 or higher: 34 components (21%)
- Score 750-850: 21 components (13%)
- Score 750 or lower: 106 components (66%)

Components with a score of 750 or lower are likely to be unregistered compounds, so in this example, 66% of the analytes measured are possibly not registered in the database.
msFineAnalysis offers correct molecular formula and structural information even if the component is not registered in the library.

Integrated Analysis of Fatty Acid Methyl Esters (FAMEs) by using GC/TOFMS (MSTips No.301)

The composition of fatty acids in fat (triacylglycerols) can be obtained by hydrolyzing the fat, derivatizing the resulting fatty acids to methyl esters, and measuring the methyl esters by GC-MS.

Polyunsaturated fatty acids such as eicosapentaenoic acid(EPA) and docosahexaenoic acid(DHA) are crucial components in biochemistry, but the methyl ester molecular ions are not detectable with EI. However, FI is most suitable for determining the molecular weight of polyunsaturated FAMEs.
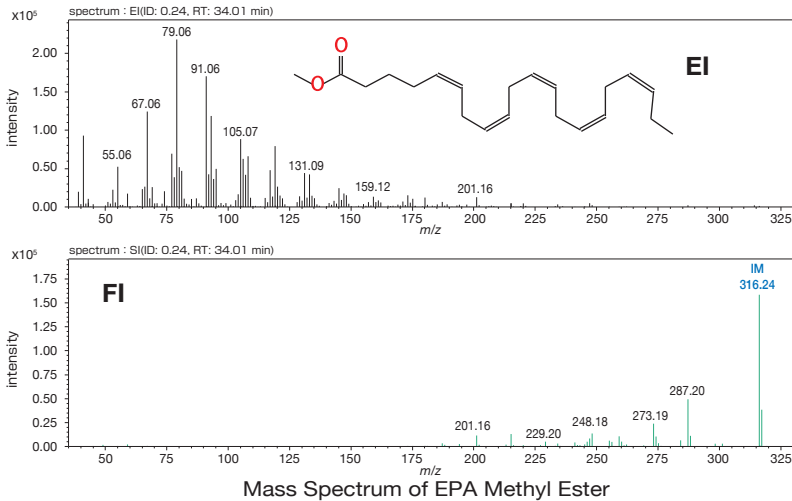
A commercial standard solution containing 37 FAMEs (Restek Corporation, 200-600 ng/uL) was measured, and the molecular ions for all components were observed in the FI mass spectra as the base peak, even for the EPA methyl ester with 5 double bonds in the alkyl group.

Consequently, msFineAnalysis can be used to automatically integrate the molecular formula results from FI with the library search results from EI to identify FAMEs.

Mass Spectrum of EPA Methyl Ester

Integrated Analysis Results for 37 FAMEs

Integrated Analysis of Coffee Aroma Component using HS/GC-TOFMS (MSTips No.280)

Headspace (HS)/GC-MS analysis is a common method for measuring volatile components in a sample. This method involves placing liquid or solid sample in a sealed vial, heating the sealed vial, and then sampling the headspace volatile components for GC-MS analysis.

For this example, 10 mL coffee liquid sampled immediately after preparation was measured by HS/GC-TOFMS. Afterwards, the msFineAnalysis integrated analysis was used to identify 67 aroma components. The characteristic volatiles from coffee - adehydes, furans, and pyrazines - were confirmed.

msFineAnalysis is also very useful for analysis of aroma components.

Integrated Analysis Result of Coffee Aroma Components

Applications using AccuTOF™ GC-Alpha

Condensation polymers such as polyesters have complicated pyrolysis processes and produce various pyrolysates. Therefore, it can be difficult to analyze the data, and structural analysis of the original polymer is sometimes not possible. In such a case, adding a derivatization reagent to perform reactive pyrolysis GC-MS is useful.

We conducted pyrolysis GC-MS of FRPC (Flame Retardant Polycarbonate) containing tetrabromobisphenol A, a typical flame retardant for aromatic polymer materials. By comparing the pyrolysis result of FRPC only and the reactive pyrolysis result for a mixture of FRPC and tetramethylammonium hydroxide (TMAH), a methylation reagent, we were able to determine the structure of the end group. The component structures shown on the TICCs were determined from the accurate mass EI mass spectra.

(A) FRPC structure (repeating portion only)
(B) Structure containing the end group as determined from the analysis results
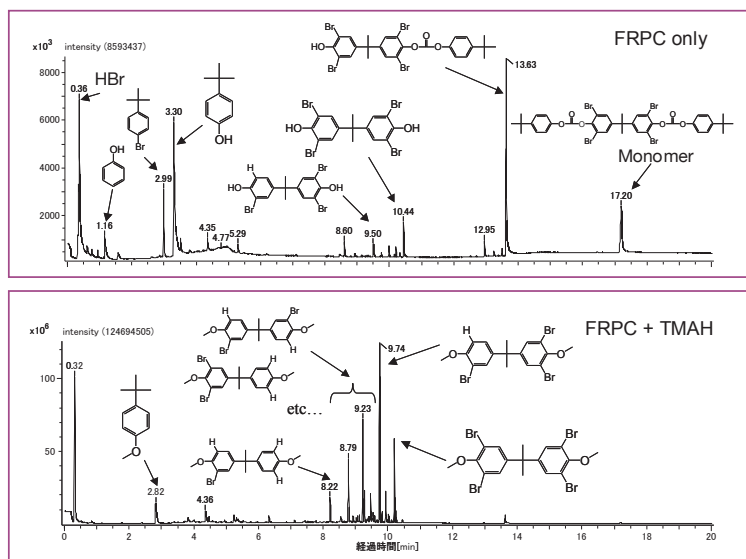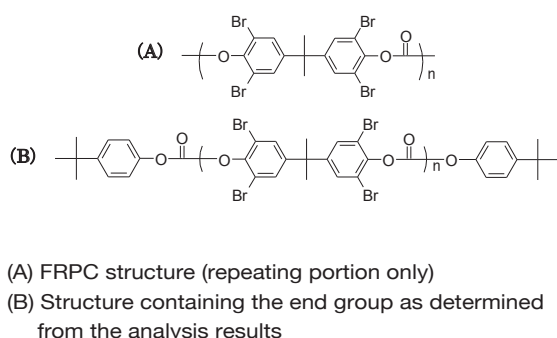
TICCs of Pyrolysis/GC-MS of FRPC and Reactive Pyrolysis/GC-MS

Analysis of a Fluorinated Compound

Many fluorinated compounds show no molecular ions with EI. With CI, some fluorinated compounds show a hydride-abstracted cation [M-H]+, which can be easily misinterpreted as a protonated molecule [M+H]+. With FI, the molecular ion M+· can be clearly observed.
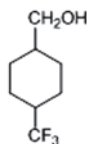
4-(Trifluoromethyl) cyclohexanemethanol
$C_8H_{13}F_3O$
Mw : 182.09185
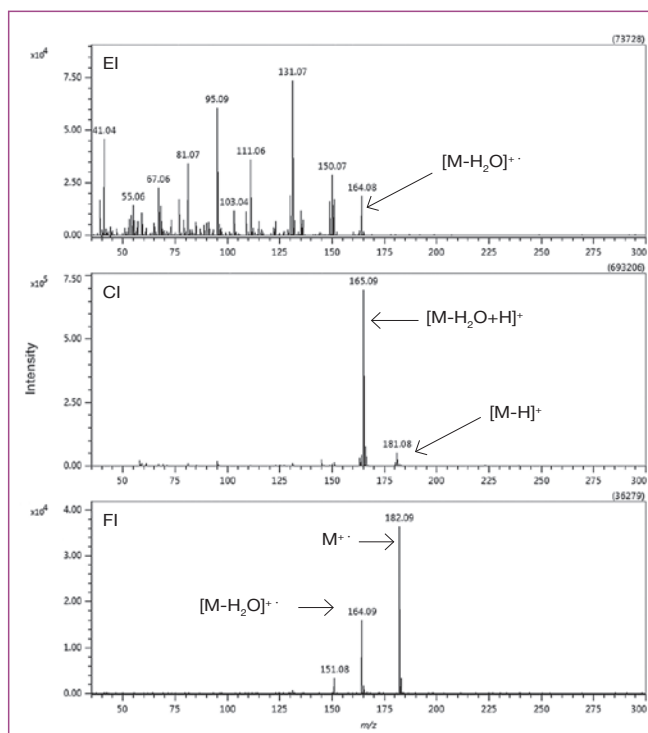
Mass spectra of a fluorinated compound

Analysis of a High-Boiling-Point Compound (Antioxidant) (MSTips No.123)

Because FI does not ionize column bleed, the TICC clearly shows the high-boiling-point compounds.
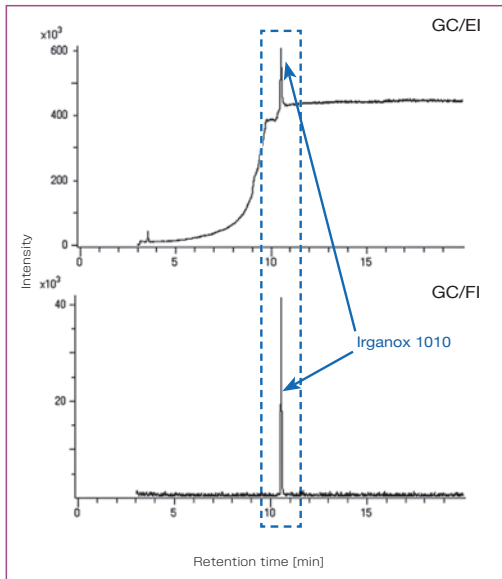
TICC of Irganox1010(antioxidant)

Irganox1010
$C_{73}H_{108}O_{12}$ Mw: 1176
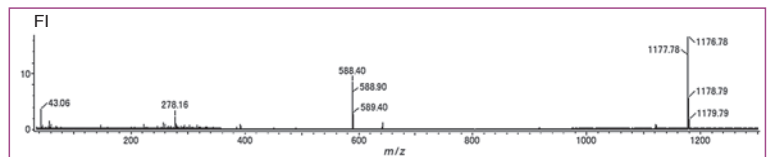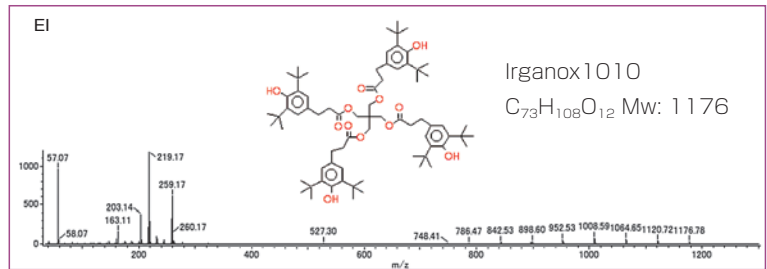
* Irganox is a registered trademark of BASF SE.

High quality GC-MS interface with no cold spot

Irganox 1010 is one of the highest boiling point compounds amenable to GC-MS. The total ion current chromatogram of Irganox 1010 shows a sharp, symmetric chromatographic peak, thus supporting the thermal homogeneity of the GC-MS interface.

Analysis Using Nitrogen as GC Carrier Gas (MSTips No.317)

Helium is ideal as a carrier gas for non-target analysis by GC-MS because it is an inert gas with a low molecular weight. However, it is expensive and can be difficult to get for some researchers. Hydrogen gas has also been used as an inexpensive GC carrier gas, but it is known to react with some compounds in the GC injection port, thus making it unsuitable for non-targeted analysis of unknowns. Nitrogen is an inexpensive inert gas that is suitable for non-targeted analysis. However, with a conventional EI ion source, the sensitivity is reduced when compared to the results for helium.

The AccuTOF™ GC-Alpha EI/FI combination ion source is an open type ion source, meaning that it does not have an enclosed ionization chamber. When it is used with nitrogen as the carrier gas in EI mode, the sensitivity is only slightly decreased when compared to helium as the carrier gas. Moreover, because nitrogen is not ionized in FI mode, the sensitivity is unchanged when compared to the results from helium.

Using the EI/FI combination ion source for Py/GC-MS analysis of acrylic resin, an equivalent result is obtained in terms of sensitivity and GC separation.
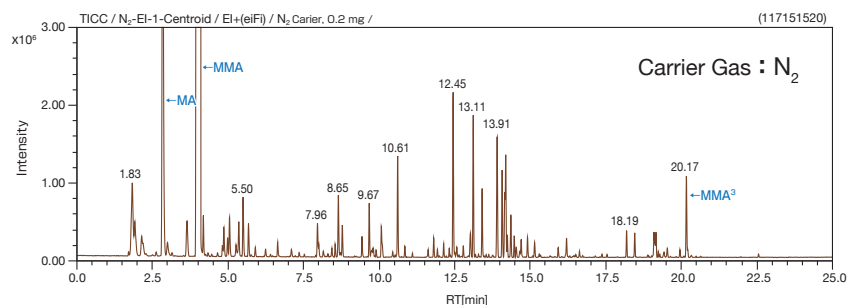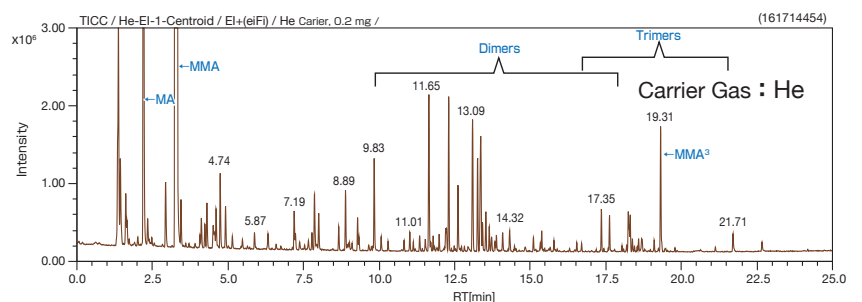
Comparison of TICC when acrylic resin is analyzed using Py-GC-TOFMS.
Ion source: EI/FI combination ion source   Ionization method: EI

Applications using AccuTOF™ GC-Alpha

GCxGC-TOFMS Analysis of Tea Tree Oil   (MSTips No.233)

The compounds in an aroma oil were fully separated for grouping. The data offers a visual representation of the complex aroma oil composition.

For compounds that do not produce molecular ions by EI, FI can be used to detect the molecular ions and determine their elemental compositions, which enhances the accuracy of qualitative analysis.
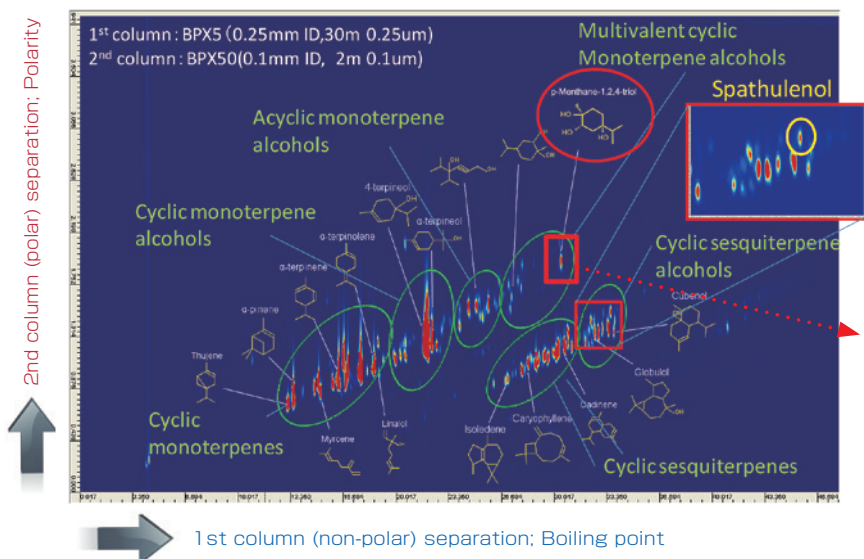
2D TICC of tea tree oil by GCxGC/TOFMS
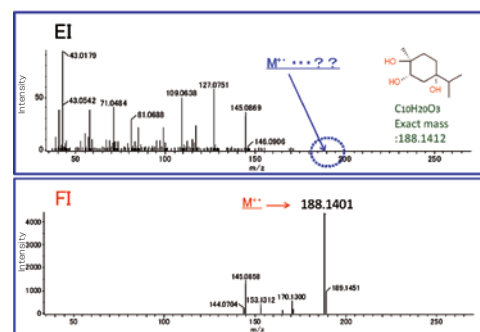
Analysis of Isomeric Disaccharides *

Methyloxime-trimethylsilyl(TMS) derivatives of disaccharides are very easy to fragment, thus making it difficult to observe molecular ions with EI or protonated molecules with CI. FI produces abundant molecular ion as well as structurally informative fragment ions to differentiate isomers.

Maltose
Glu-Glu (1-4)
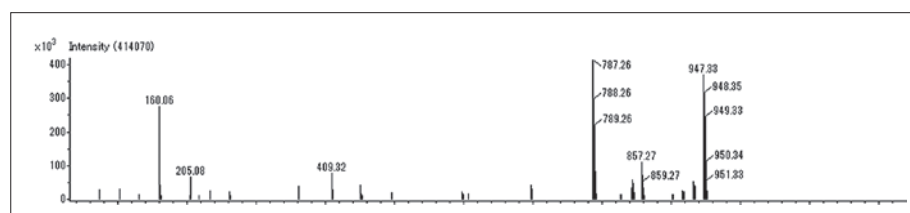
FI mass spectrum of the methyloxime-TMS derivative of maltose

Laminaribiose
Glu-Glu (1-3)
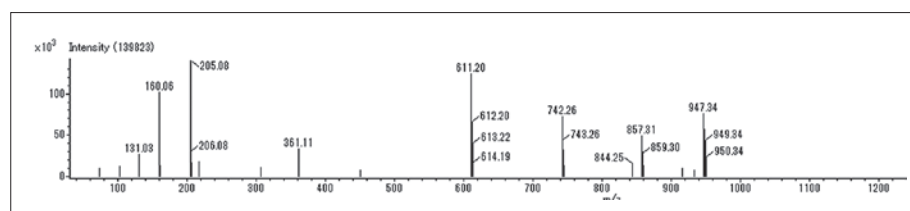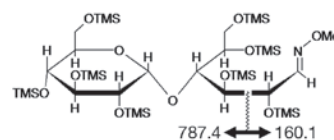
FI mass spectrum of the methyloxime-TMS derivative of laminaribiose
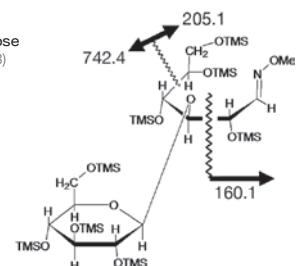
* Furuhashi, T. & Okuda, K. Critical Rev. Anal. Chem., 1 - 16, doi:10.1080/10408347.2017.1320215 (2017).
  Disaccharide TMS derivative: Courtesy of Tsuyoshi Furuhashi, Anicom Specialty Medical Institute Inc.

Analysis of Agrochemical Residues in Food (MSTips No. 142, 143, 144)

■ High selectivity

High-resolution TOFMS can reduce interference from matrix. Peaks from the matrix that are detected at low resolution can be eliminated at high resolution. This high selectivity reduces false positives and allows for more accurate quantitation.
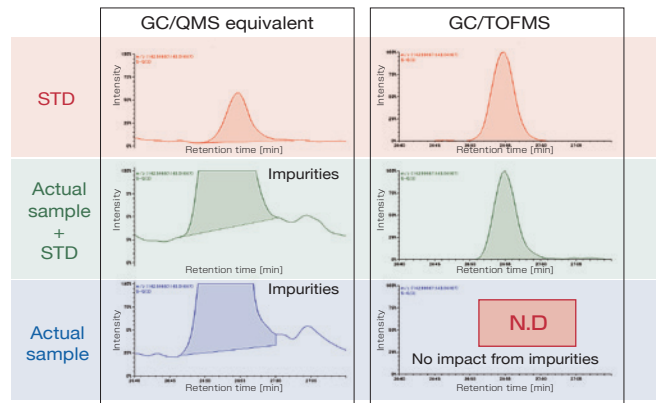
Extracted Ion Chromatogram (EIC) of Agrochemical Component in Carrot Sample

■ Simple analytical conditions

GC/TOFMS detects all components that are ionized. Thus, the operator is freed from the lengthy process of defining analytical conditions such as SIM (Selected Ion Monitoring) and SRM (Selected Reaction Monitoring). Theoretically, there is no limit on the number of components that can be analyzed. The AccuTOF™ GC-Alpha can perform simple simultaneous analysis of multiple components using its unique exact mass database for approximately 350 components (1 quantitative ion and 4 qualitative ions per component, editable).

■ Superior qualitative capability

TOFMS performs high-resolution, high-mass-accuracy analysis over a wide m/z range (m/z 35 to 600) without selecting a measurement mode such as SCAN and SIM. As a result, it allows for acquisition of highly selective chromatograms for all ions observed, demonstrating its superior qualitative capability. The acquired data can be used to analyze non-target compounds as well.

■ Superior sensitivity/reproducibility

The table on the right shows the limit of quantitation and the relative standard deviation of 353 components that were analyzed simultaneously. The results demonstrate superior sensitivity and reproducibility for simultaneous analysis of multiple components.

Limit of quantification(LOQ)		%RSD	
< 0.005ppm	161	< 5%	239
0.005ppm - 0.01ppm	174	5 ～ 10%	109
> 0.01ppm	18	>10%	5

*LOQ defined as 10 times the standard deviation of the quantitation values obtained from 5 repeated injections of 40 pg (20 ppb x 2 µL) of each compound.

■ High-throughput analysis - FastGC

These chromatograms show the presence of 100 pesticide components. In the Fast GC analysis (top), the system acquired data while maintaining chromatographic separation in less than 1/4 of the time needed for the conventional analysis (bottom). The 50 spectra/second high-speed data acquisition system enables high-throughput analysis.
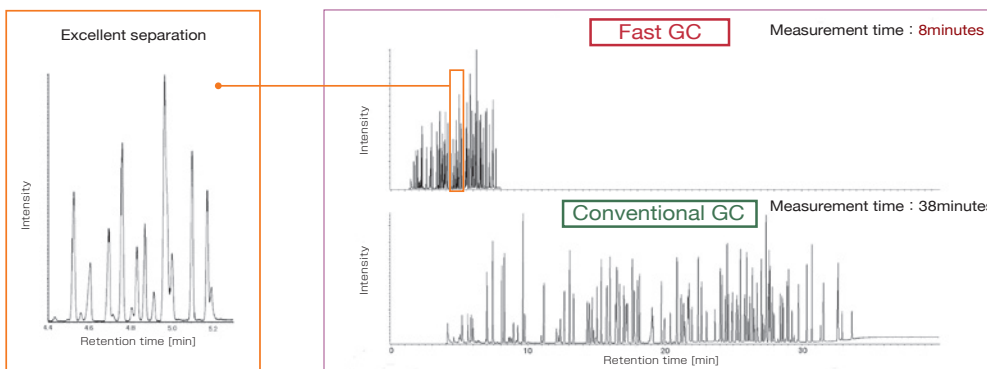
AccuTOF™ GC-Alpha **with Direct MS**

Direct MS mode is useful for the analysis of high-boiling-point and high-mass compounds that are not amenable for GC

TOFMS with inherent **wide mass range** is **well-matched** with direct MS mode.

Compounds that are measured by GC normally have molecular weights below 500Da, so it is not common to target compounds with molecular weights exceeding 1000Da by using GC-MS. However, in direct MS mode (no GC is used), high-boiling-point, high-molecular-weight, and nonvolatile compounds can be targeted for measurement, as the sample is directly introduced into the ion source. The mass range of the AccuTOF™ GC-Alpha is *m/z* 6,000 or higher. Since compounds can be detected over a wider mass range than conventional GC-MS, the system is well suited for measurements in direct MS mode.

Three Direct MS Probes To Choose From

■ DEP (Direct Exposure Probe)

Platinum filament

▶ Sample dissolved or dispersed in solvent is applied to the filament at the tip
▶ Suitable for high boiling point and/or thermally labile compounds
▶ Compatible with EI and CI

■ DIP (Direct Insertion Probe)

Glass sample tube

▶ Solid sample can be introduced in the glass sample tube
▶ Suitable for high boiling point and/or insoluble compounds
▶ Compatible with EI and CI

■ FDP (Field Desorption Probe)

Carbon Emitter

▶ Sample dissolved or dispersed in solvent is applied to the carbon emitter at the tip
▶ Suitable for high boiling point, high molecular weight, and/or thermally labile compounds
▶ Suitable for low- to mid-polar metal complexes
▶ Used for FD soft ionization

Load-lock flange for DIP/DEP/FDP

Analysis of Pigments by FD

Samples such as pigments that are insoluble in solvent can be measured by using FD. Molecular ions are clearly detected in the FD mass spectra.

$\times 10^5$ 1.00

Copper(II)phthalocyanine(α-form)
$C_{32}H_{16}CuN_8$
Most Abundant mass : 575.08

575.08

$\times 10^4$

Pigment Green 7
$C_{32}Cl_{16}CuN_8$
Most Abundant mass : 1126.44

1126.44
562.23
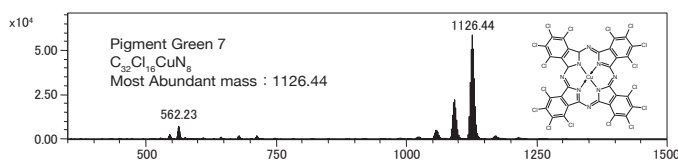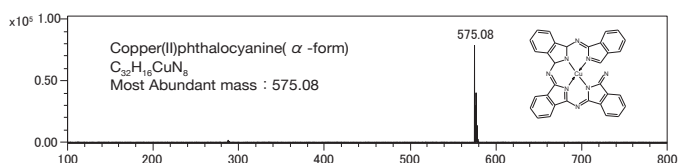
FD mass spectra of pigments

FD Sampling Tool

A dedicated sampling tool makes it easy to apply sample solution directly on to the FD emitter.

FD Sampling Tool

Polymer Analysis by FD and Kendrick Mass Defect (KMD) Analysis

FD is an ionization method in which the analyte molecules applied to the emitter are desorbed and ionized by a high electric field. The electric current running through the emitter is gradually increased during the measurement to heat the analyte to assist desorption/ionization. Since the optimum emitter current for ionization depends on the analyte, components can desorb at different times. Separation of components in a mixture is possible, and mass spectra for a specific class of compounds can be extracted. Furthermore, even when compounds ar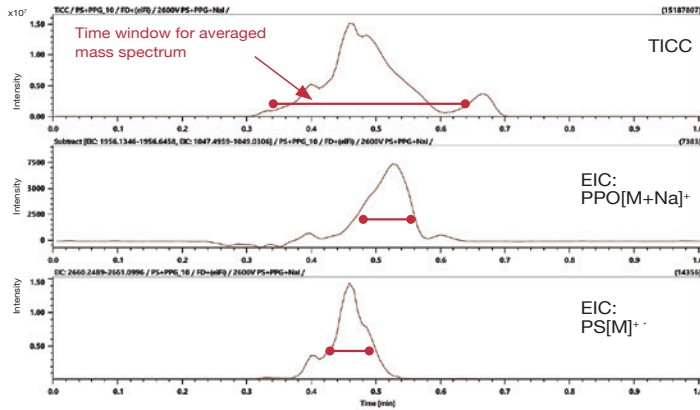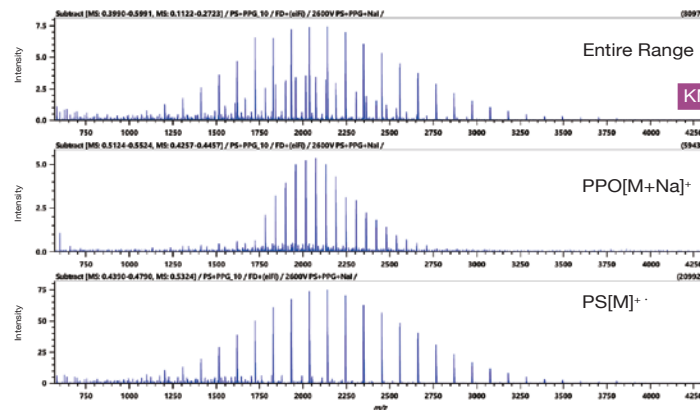e not separated in time during desorption/ionization, each other, target components can still be clearly separated by creating KMD plots.
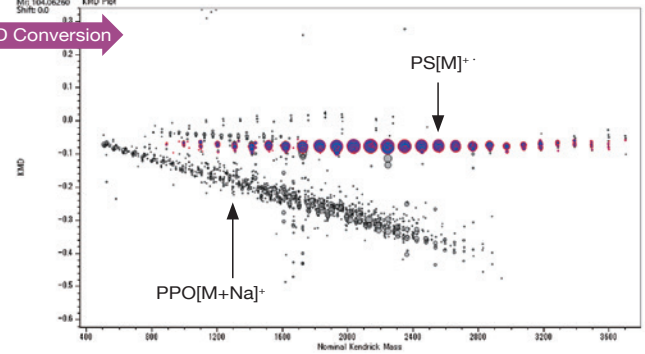

FD Measurement Data

FD Mass Spectra

KMD Conversion

KMD plot for the entire range mass spectrum

Type Analysis using **msRepeatFinder**
– Calculation of the sum of intensities and average molecular weights –

msRepeatFinder can analyze polymers and hydrocarbons, which are composed of repeating units, by visualizing complex mass spectra with KMD plots. The figure on the right shows KMD plots for a FD mass spectrum of crude oil. By visualizing hydrocarbons of different degree of unsaturation, analysis and grouping of each series becomes an easy task.

Moreover, by grouping each series, a type analysis calculation can automatically be performed for each group that includes:

▶ Sum of Intensities
▶ Number Average Molecular Weight
▶ Weight Average Molecular Weight

Detailed type analysis is possible by visualizing spectra with KMD plots.

KMD Plot of Crude Oil
Left: All, Right: Grouping of hydrocarbons of Unsaturation Degree 0-9
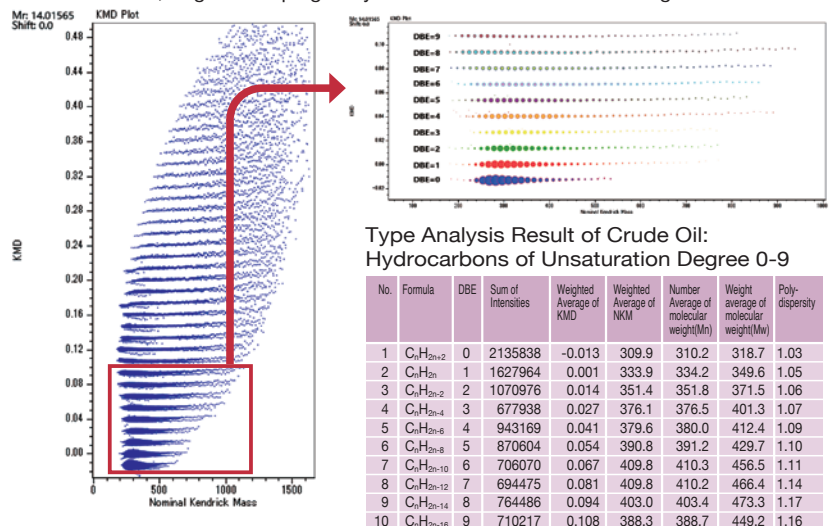
Type Analysis Result of Crude Oil:
Hydrocarbons of Unsaturation Degree 0-9

No.	Formula	DBE	Sum of Intensities	Weighted Average of KMD	Weighted Average of NKM	Number Average of molecular weight(Mn)	Weight average of molecular weight(Mw)	Poly-dispersity
1	C_nH_{2n+2}	0	2135838	-0.013	309.9	310.2	318.7	1.03
2	C_nH_{2n}	1	1627964	0.001	333.9	334.2	349.6	1.05
3	C_nH_{2n-2}	2	1070976	0.014	351.4	351.8	371.5	1.06
4	C_nH_{2n-4}	3	677938	0.027	376.1	376.5	401.3	1.07
5	C_nH_{2n-6}	4	943169	0.041	379.6	380.0	412.4	1.09
6	C_nH_{2n-8}	5	870604	0.054	390.8	391.2	429.7	1.10
7	C_nH_{2n-10}	6	706070	0.067	409.8	410.3	456.5	1.11
8	C_nH_{2n-12}	7	694475	0.081	409.8	410.2	466.4	1.14
9	C_nH_{2n-14}	8	764486	0.094	403.0	403.4	473.3	1.17
10	C_nH_{2n-16}	9	710217	0.108	388.3	388.7	449.2	1.16

Pre-treatment Device for Various Experimental Needs

Pyrolysis

A Pyrolyzer (Py) is valuable for the analysis of materials as a pre-treatment device that enables GC-MS measurement of solid samples such as polymers.

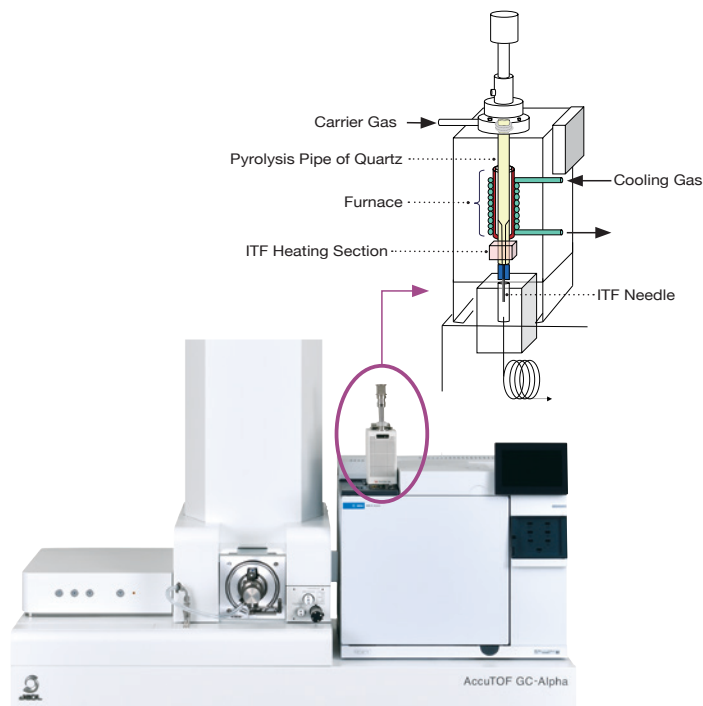By heating a sample in the pyrolyzer furnace, components such as

▶ Volatile components evolved from the sample
▶ Thermal decomposition products of the sample

are released. These released components are then analyzed by GC-MS for additional information about the sample.

Because a sample is placed in a small metal cup for analysis, solid and liquid sample analysis is possible as long as the sample can fit inside the cup. Since this technique was originally developed to perform structural analysis of polymer materials, the sample volume for the analysis is typically small.

By attaching the Frontier Laboratories Ltd. multi-functional pyrolyzer, both pyrolysis for structural analysis of polymer materials as well as direct analysis of evolved gases (Evolved Gas Analysis: EGA) for finding the optimal pyrolysis temperature are possible.
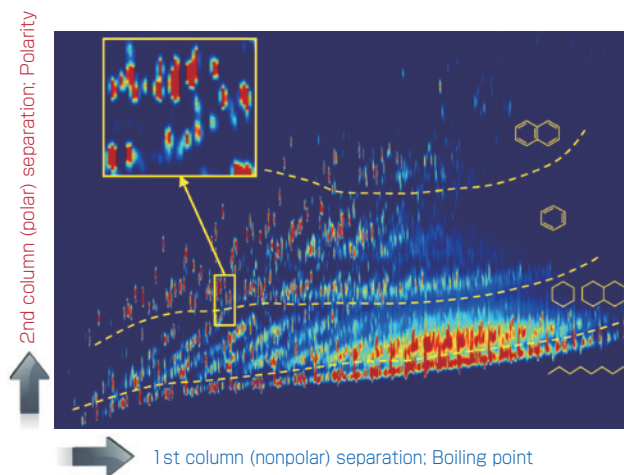
Optional attachments include the Micro Jet Cryo Trap which is a selective sample introduction device that allows for more sophisticated analyses using EGA/heart cut/GC-MS in which the gas components evolved from a specific temperature range are measured by GC-MS.

Carrier Gas
Pyrolysis Pipe of Quartz
Cooling Gas
Furnace
ITF Heating Section
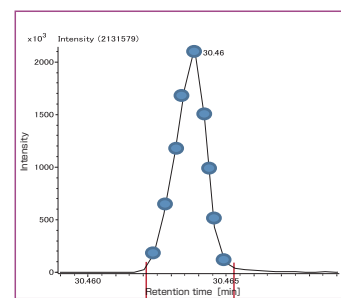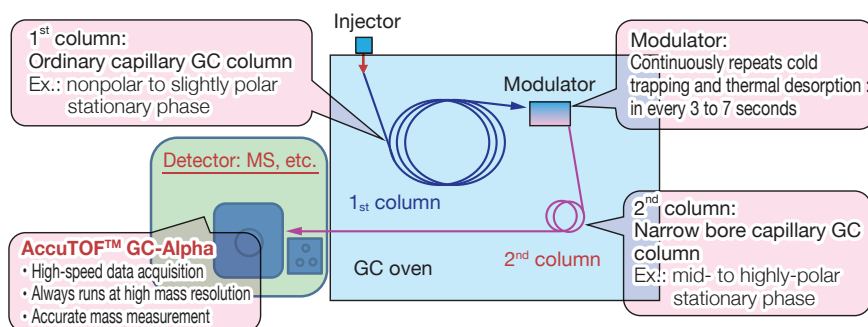ITF Needle

AccuTOF GC-Alpha

GC x GC (Comprehensive 2D GC)

GCxGC is an ultrahigh-separation chromatography system that uses 2 GC columns with different polarities in series. The eluted components from the 1st column are trapped and then released at specified intervals into the 2nd column using a modulator between the two columns. High-speed data acquisition is used to detect the components separated by the 2nd column. GCxGC is a powerful capillary GC technique that features higher resolution chromatography than traditional capillary GC and is capable of high-sensitivity group analysis of sample components. This technique requires a detector capable of high-speed data acquisition because the peak widths in the chromatograms are extremely sharp compared to traditional capillary GC.

The AccuTOF™ GC-Alpha enables accurate mass measurement using EI, FI, PI, and CI methods, while acquiring as many as 50 spectra per second. This is especially effective for nontargeted qualitative analysis of trace components.

2nd column (polar) separation; Polarity

1st column (nonpolar) separation; Boiling point

2-dimensional (2D) TICC of diesel fuel by GCxGC/TOFMS

1st column:
Ordinary capillary GC column
Ex.: nonpolar to slightly polar stationary phase

Injector

Modulator:
Continuously repeats cold trapping and thermal desorption : in every 3 to 7 seconds

Modulator

Detector: MS, etc.

1st column

AccuTOF™ GC-Alpha
· High-speed data acquisition
· Always runs at high resolution
· Accurate mass measurement

GC oven

2nd column

2nd column:
Narrow bore capillary GC column
Ex.: mid- to highly-polar stationary phase

×10³ Intensity (2131579)
Intensity
2000
1500
1000
500
0
30.46
30.460   30.465
Retention time [min]

Peak width: 0.18 s

9 data points

Thermogravimetry / Differential Thermal Analysis (TG/DTA)

TG and DTA are related techniques that evaluate physical properties of a material using heat. TG focuses on sample weight changes during sample heating, while DTA focuses on changes in the sample itself relative to a reference material. In each case, a more detailed evaluation of these changes can be done by measuring the components that are released from the material as the weight changes in real-time by using MS.

Measuring accurate mass of molecular ions obtained by soft ionization enables estimation of elemental compositions of organic compounds generated through thermal decomposition.

Also, for the analysis of generated gases, the high mass resolution allows independent monitoring of the time dependence for isobaric ions such as $CO^+/N_2^+/CH_2N^+/C_2H_4^+$, which have the same nominal mass of 28 Da.

■ Thermal Analysis of Fluorocarbon Polymers (MSTips No.249)

A number of high-mass ions with specific repeat units were observed around m/z 2,500 that indicate the thermal decomposition of the fluorocarbon polymer. The TG-TOFMS data showed peaks in the range above m/z 1000 which is higher than the typical TG-QMS which makes it ideal for the measurement of synthetic polymers.
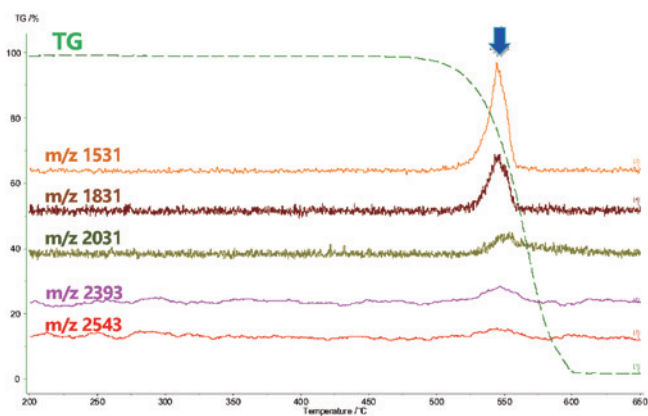
TG curve and EIC chromatograms for high m/z ions
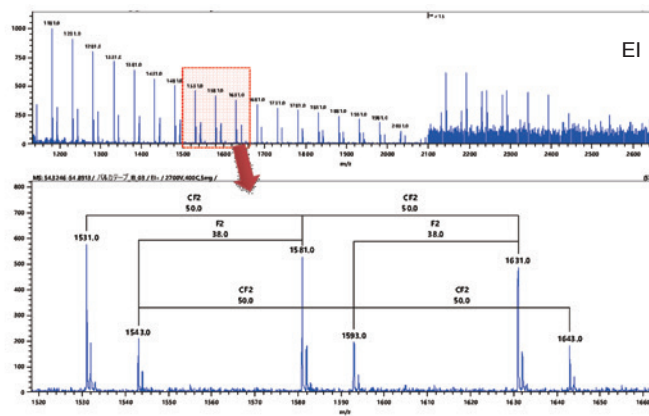
EI Mass Spectrum of position indicated by blue arrow mark in TG curve
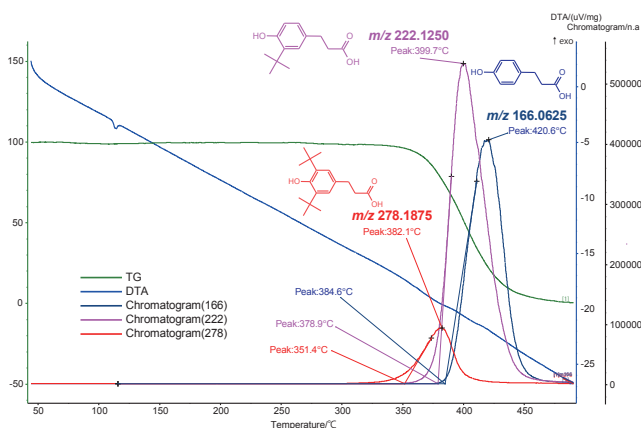
■ Thermal Decomposition Analysis of Antioxidant Additive (MSTips No.250)

Based on their accurate mass analysis, the ions observed at m/z 166, 222, and 278 were determined to have structures derived from the thermal decomposition of an antioxidant.

With TG-MS and no chromatographic separation, the combination of soft ionization and accurate mass measurement, a feature of TOFMS, allows the qualitative analysis of multiple components that are not separated in time. TG-TOFMS is a powerful analytical tool for the detailed thermal analysis of synthetic polymers and additives.
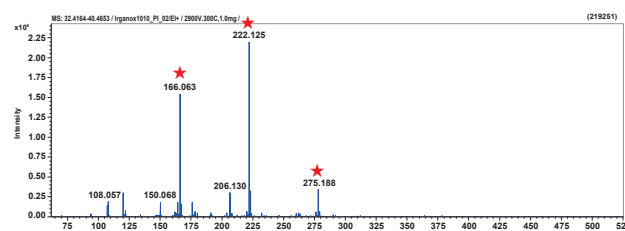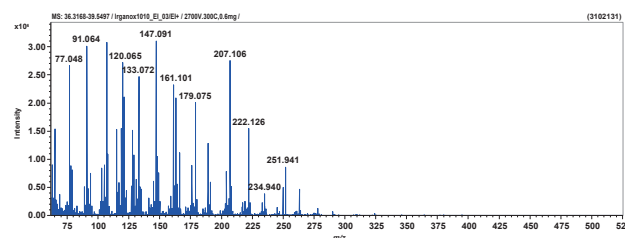
Mass	Formula	Calculated Mass	Mass Difference [mDa]	DBE
166.0625	$C_9 H_{10} O_3$	166.0625	0.1	5
222.1250	$C_{13} H_{18} O_3$	222.1251	-0.1	5
278.1875	$C_{17} H_{26} O_3$	278.1877	-0.1	5

TG/DTA curves and EIC chromatograms for the thermal decomposition products of the antioxidant

EI, PI Mass Spectrum and PI Accurate Mass Analysis Result (★ mark in the figure)

Software to expand the range of applications

Main Program - msAxel

■ Auto Tuning

▶ Accomplishes high performance tuning without a lengthy manual adjustment process.
▶ Easily achieves optimum sensitivity and resolution in all ionization modes (EI, CI, FI, FD, PI).

■ Powerful Automated Functions

▶ Auto Drift Correction
   Automatically performs drift correction for every spectrum in the measured data
▶ Auto Data Conversion
   Automatically converts measured data to netCDF format.
▶ Auto Data Transfer
   Automatically transfers acquired data to any storage or archival location (external PC for data analysis, etc.)
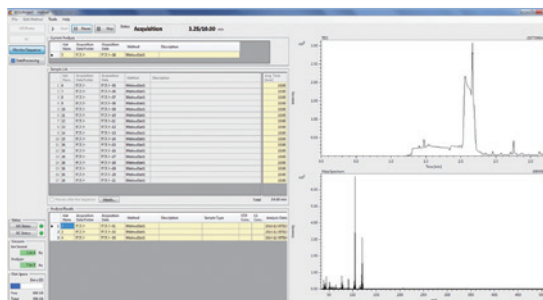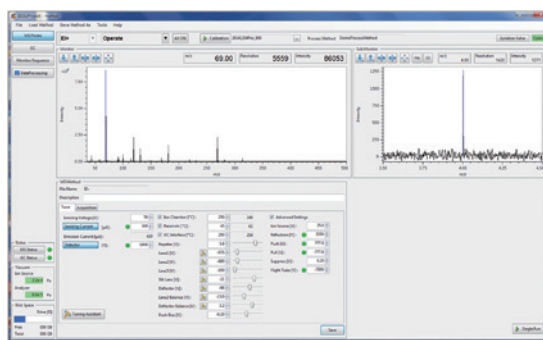

Optional Multicomponent Quantitative Analysis Program - Escrime™

Escrime™ is designed to calculate EIC peak areas, plot calibration curves, and determine quantitative values for a large number of target components all at once. A narrow "*m/z* window width" can be set to generate EICs for quantitation that take full advantage of the high mass resolving power of the AccuTOF™ GC-Alpha. This software significantly speeds up the quantitative analysis process by allowing further data manipulation by separate or collective editing of peak area calculation ranges.

Peaks for components contained in multiple samples or peaks for multiple components in an individual sample can be displayed in a single view.
The peak area calculation ranges can be simultaneously changed, allowing for batch analysis of more than 150 samples.
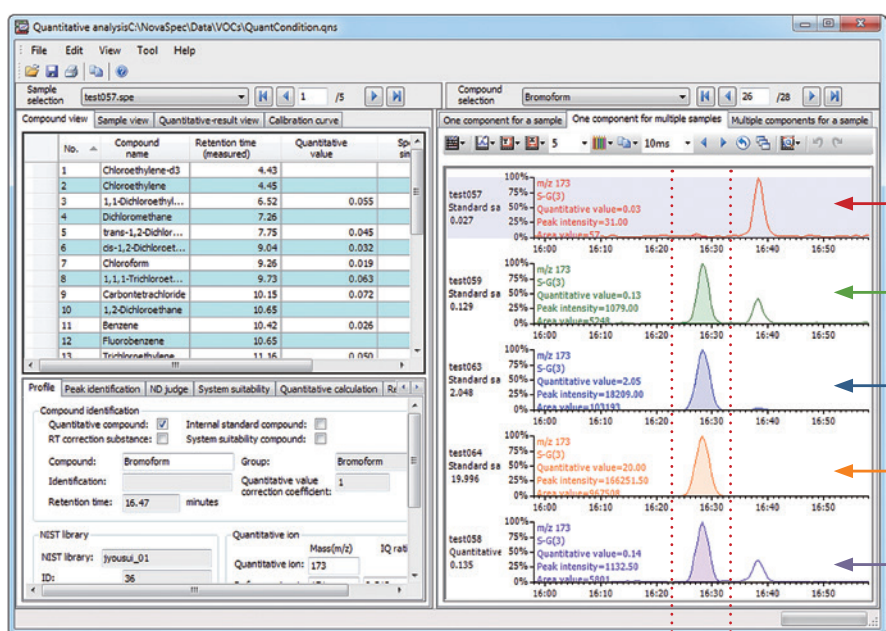
Repeating Structure Analysis Program – msRepeatFinder (option)

■ Definitive Polymer Analysis Software

Visualizes complicated mass spectral data and accelerates information sharing

▶ Imports and display peak lists
Up to 10 lists can be overlaid

▶ KMD plots
Nominal Kendrick Mass vs. Kendrick Mass Defect

▶ KMR (Kendrick Mass Remainder) plots
Kendrick Mass Remainder vs. Kendrick Mass Defect

▶ Fraction base KMD plots

▶ RKM (Remainder of Kendrick Mass) plots
Nominal Kendrick Mass vs. Remainder of Kendrick Mass

▶ Estimated circles of homopolymer end groups (on KMR plots)

▶ Grouping
· Color coded groups
· Enable/disable display of polymer series groups
· Calculating average molecular weight/polydispersity of groups
· Export polymer series groups
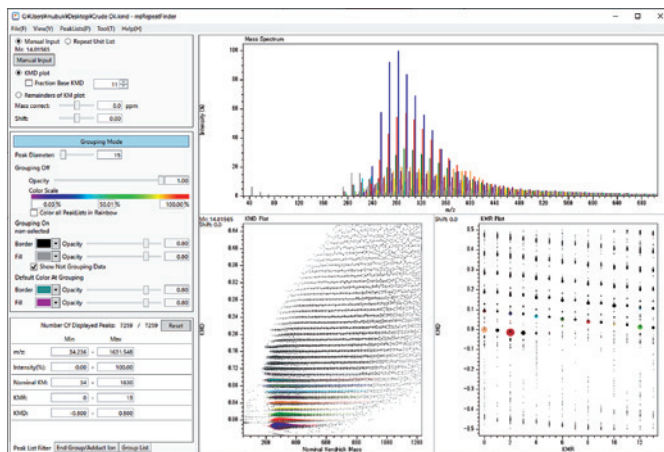
Optional Type Analysis Program for Polymers and Hydrocarbons - Polymerix

FD generally forms ions that reflect the molecular weights of analytes through the formation of $M^{+\cdot}$, $[M+H]^+$ and $[M+Na]^+$, thus allowing for the calculation of the average molecular weight, degree of polymerization, and polydispersity from the *m/z* and the intensity of each peak. Polymerix is designed to calculate the average molecular weight, degree of polymerization, and polydispersity of polymers, and estimate the repeat structure and end groups from the data acquired in FD and FI. Moreover, this software enables type analysis of hydrocarbons measured in FD, and GC/FI, by specifying CH_2 as the repeating unit.

The example below is a visualization of the relative abundance (distribution) of each molecule in an ethylene oxide/propylene oxide (EO/PO) block copolymer.
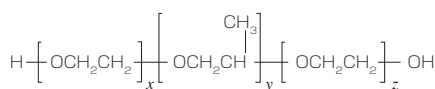
EO/PO Block Copolymer
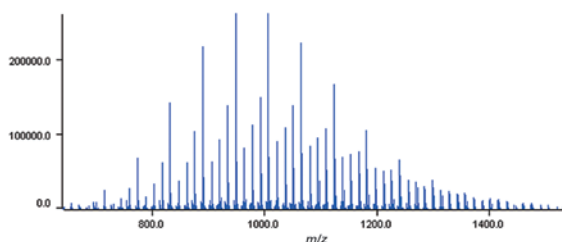
FD Mass Spectrum of EO/PO Block Copolymer

Repeat A PO: $(C_3H_6O)_n$ \ Repeat B, EO: $(C_2H_4O)_n$	0	1	2	3	4	5	6	7	8	9	10	11
6												
7												
8												
9					1.08	1.66	1.27	1.33	1.61			
10			1.63	2.17	4.19	4.24	3.04	2.26	2.58	1.72		
11	2.65	3.42	5.09	6.17	8.20	7.60	5.81	4.63	4.34	2.42		
12	9.58	10.37	12.54	14.00	15.99	13.09	9.23	5.62	4.32	3.27	2.19	1.40
13	25.98	23.80	23.46	24.20	23.93	17.79	12.39	7.36	6.81	3.56	2.24	1.22
14	54.36	39.41	35.20	31.16	26.41	20.61	13.98	9.37	7.03	4.81	2.82	1.11
15	83.18	52.75	43.08	34.49	28.19	19.84	14.31	9.97	6.35	2.97	2.14	1.09
16	99.99	56.93	41.44	32.28	25.35	18.00	12.60	8.69	6.50	3.50		
17	100.00	52.72	36.53	26.54	20.38	14.20	10.73	6.67	3.61			
18	84.89	41.17	27.92	20.53	16.96	9.92	7.72	4.55	3.09	1.37		
19	63.64	29.20	19.25	14.66	10.89	7.26	4.05	3.16	1.73			
20	40.33	19.86	13.74	9.46	6.85	4.96	1.56	1.69				
21	25.17	11.41	8.93	5.77	4.50	3.04	2.11					
22	14.63	7.35	3.67	3.55	2.94							
23	7.94	4.08	1.86									
24	4.44	2.56										
25	1.69											
26												

Mn	Mw	Mz	PD
1053.2	1077.1	1100.9	1.0

Mn : Number Average Molecular Weight
Mw : Weight Average Molecular Weight
Mz : Z Average Molecular Weight
PD : Multidispersity（Mw/Mn）

Molecular distribution of EO/PO block copolymer

JEOL Mass Spectrometer Line-up

Gas Chromatograph Quadrupole Mass Spectrometer
JMS-Q1500GC UltraQuad™ GC/MS

This is a gas chromatograph – quadrupole mass spectrometer that achieves the highest sensitivity in its class. Realizing high sensitivity by using a high-precision hyperbolic quadrupole analyzer, the JMS-Q1500GC is used in a variety of fields such as environment, food, and chemical products. The PI ion source is also available as an option, enabling the analysis of various samples such as polymer materials, additives, and gases evolved from batteries and materials. Direct MS probes are also optionally available for the analysis of nonvolatile materials.

Gas Chromatograph Triple Quadrupole Mass Spectrometer
JMS-TQ4000GC GC-MS/MS

Building upon the features of the JMS-Q1500GC, the JMS-TQ4000GC is a gas chromatograph – triple quadrupole mass spectrometer 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 function in the short collision cell and instantaneous ejection of accumulated ions provides high sensitivity and high selectivity even in high-speed SRM measurements.

MALDI-TOFMS

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

The JMS-S3000 SpiralTOF™-plus is a matrix-assisted laser desorption/ionization – time-of-flight mass spectrometer (MALDI-TOFMS) with ultrahigh resolution and high sensitivity, by using our unique 17-meter SpiralTOF™ ion optics system. The JMS-S3000 has evolved into the SpiralTOF-plus with greatly enhanced mass imaging capabilities. This model is at the forefront of MALDI analytical technology and satisfies the ever-changing research needs for a wide range of fields including synthetic polymers, materials science, and biopolymers.

LC-MS, DART-MS

Atmospheric Pressure Ionization
– Time-of-Flight Mass Spectrometer
JMS-T100LP AccuTOF™ LC-plus 4G

The latest generation in this award winning series, the JMS-T100LP AccuTOF™ LC-plus 4G is a simple, robust and versatile atmospheric pressure ionization – time-of-flight mass spectrometer. In addition to the electrospray (ESI) ion source, which is the most widely used ion source for LC-MS, JEOL's unique ionization technologies, DART™(Direct Analysis in Real Time) and ColdSpray provide solutions for a wide range of analyses.

Specification & Configuration

Standard Configuration

Ion Source	Electron Ionization
Analyzer	Reflectron Time-of-Flight Mass Spectrometer
Detector	Dual Micro Channel Plate
Data Acquisition System	Continuous Averager
Gas Chromatograph	Agilent 8890
Data System	Personal Computer, Monitor, Color Printer, Windows® Operation System, Main Program (msAxel), Automated Data Analysis Program (msFineAnalysis)

Major Options

- EI/FI/FD combination ion source
- EI/PI combination ion source
- CI ion source
- FD/FI ion source
- DIP
- DEP

Installation Requirements

Power Supply

Main Console	Single phase AC 190-210 V or 220-240 V, 20 A, 50-60 Hz
Gas Chromatograph	Single phase AC 200V or 220 V or 230 V or 240 V, 20 A
Data System	AC 100-120 V, 15 A, 50-60 Hz,or AC 200-240 V, 7.5 A, 50-60 Hz
Grounding	100 Ω or less

Gas

Nitrogen gas (for purging ion source and analyzer, for driving valves)
0.5 to 0.6 MPa, 97% or better purity

Helium gas (for gas chromatograph)
0.5 to 0.68 MPa, 99.999% or better purity
(0.5ppm or less hydrocarbon content)

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

Installation Room

Environmental Magnetic Field	Varying magnetic field 1×10^{-6} T or less
	Static magnetic field 5×10^{-4} T or less
Floor Vibration	Amplitude (p-p) 25μm or less
	Accelerating Voltage 0.1 m/s^2 or less
Room Temperature	20 to 27 ℃
Temperature fluctuation	±3 ℃/h or less
Humidity	30 to 70% (no condensation)
Maximum heat generation	25,776 kJ/h
	(calculated from maximum power consumptions of mass spectrometer, gas chromatograph, and data system)
Ventilation Facility	Required for rotary pump exhaust

* For details of installation requirements, please inquire a local sales office.

Standard Installation Example

Alphabet	Unit	W (mm)	D (mm)	H (mm)	Weight (kg)
A	Mass Spectrometer Basic Unit	1430	790	2480	348
B	Gas Chromatograph	580	510	490	49
C	Rotary Pumps (per unit)	232	430	225	25
D	Personal Computer	177	345	331	11
E	PC monitor	520	166	351	5
F	Color Printer	430	418	287	13

*Two rotary pumps are required.
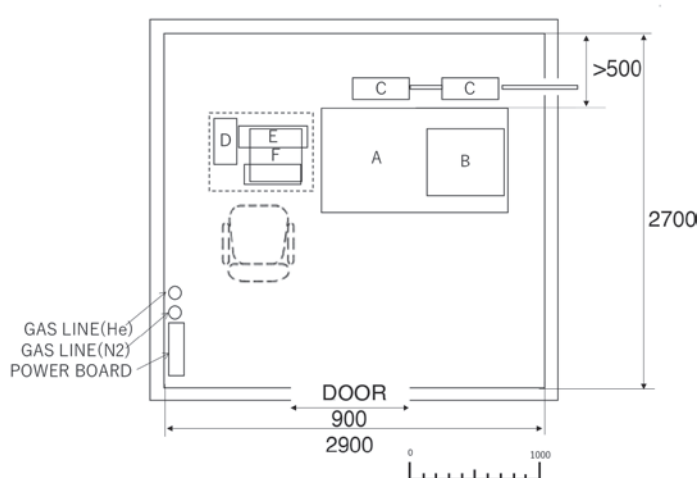
< Caution >

● To place the rotary pumps (RP) behind the basic unit, the distance from the rear of the basic unit to the room wall must be 500 mm or more.

● An exhaust duct or port is needed for the rotary pumps (RP).

● The table for PC and printer must be prepared by the customer.

● Supply gas up to primary side must be prepared by the customer.

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