



Scientific / Metrology Instruments
High Performance Gas Chromatograph Time-of-Flight Mass Spectrometer

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 the JMS-T2000GC “AccuTOF™ GC-Alpha”, the ultimate GC-MS with superior performance and ease of operation



2004

JMS-T100GC AccuTOF™ GC

- Mass resolving power $\geq 5,000$
- 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 \rightarrow 6,000)



2012

JMS-T100GCV AccuTOF™ GCv 4G

- Higher mass resolving power (6,000 \rightarrow 8,000)
- Better mass accuracy (5 ppm \rightarrow 3 ppm)
- Faster spectrum recording speed (25 Hz \rightarrow 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 \rightarrow 10,000)
- Better sensitivity (S/N 100 \rightarrow 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 three Key Technologies.



Key Technology 1

**GC-TOFMS
Technology**
(JMS-T2000GC)

2

Key Technology 2

**Soft Ionization
Technology**
(EI/FI, EI/PI, CI)

1

Key Technology 3

**AI Structural Analysis
Technology**
(msFineAnalysis AI)

3

JMS-T2000GC
AccuTOF™ GC-Alpha



Key Technology 1

New high-performance Time-of-Flight Mass Spectrometer

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.

Key Technology 2

Soft ionization methods: absolutely essential for unknown compound analysis

The following soft ionization methods are available for AccuTOF™ GC-Alpha

- ▶ CI (Chemical Ionization)
- ▶ PI (Photoionization)
- ▶ FI (Field Ionization)
- ▶ FD (Field Desorption, for direct measurement)

In particular, the FI method is the most suitable for unknown compound analysis since it is the softest ionization method available for GC-MS. A wide range of applications can be covered by selecting the appropriate soft ionization method according to the sample.

Key Technology 3

msFineAnalysis AI for automatic structural analysis

msFineAnalysis AI, an automated structure analysis software for GC-TOFMS¹⁾, is a qualitative analysis software with the following features:

1. Integrated analysis using EI and soft ionization mass spectra
2. AI-predicted EI mass spectral database
3. AI structure analysis by combining "1" and "2" above
4. Target analysis function
5. Differential analysis function

msFineAnalysis AI can support from non-target analysis to target analysis. It proposes structural formulas of unknown compounds. Innovative GC-MS qualitative analysis software is now available.

1) Only for JMS-T200GC and JMS-T2000GC



Basic Performance of AccuTOF™ GC-Alpha

High performance for both qualitative and quantitative analyses



Four “High” specifications and two “Wide” specifications achieved simultaneously

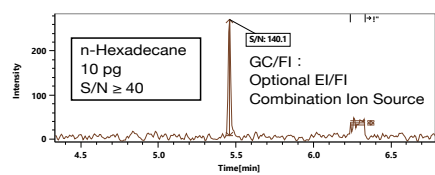
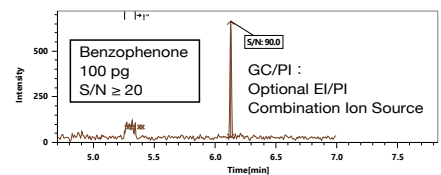
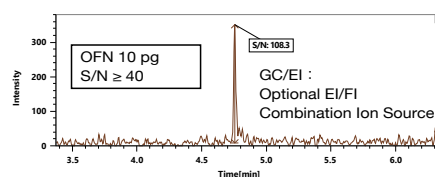
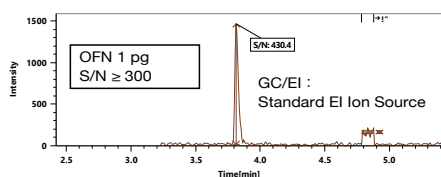
The JMS-T2000GC AccuTOF™ GC-Alpha is a high performance GC-MS system that simultaneously realizes high mass resolution, high mass accuracy, high sensitivity, high speed data acquisition, wide dynamic range, and wide mass range.

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

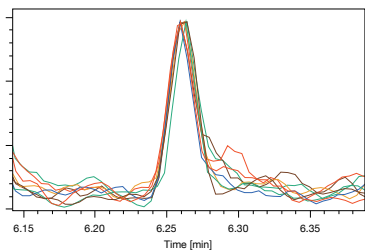
The standard EI ion source with ultra-high sensitivity is capable of micro volume trace quantitative analysis. Other ion sources are also sensitive enough for qualitative analysis and can be used in a wide range of applications.



OFN: Octafluoronaphthalene

Instrument Detection Limit: IDL = 18.7 fg

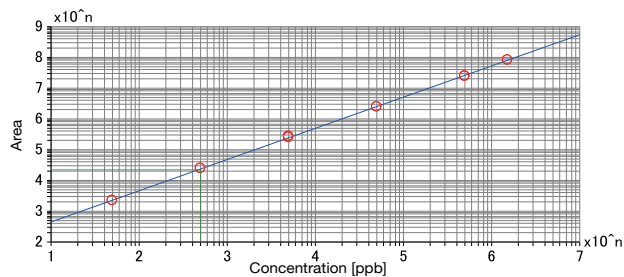
Eight sequential measurements of 100 fg of octafluoronaphthalene (OFN) were obtained by using the standard EI ion source. The instrument detection limit (IDL) is calculated based on the peak area and reproducibility of the extracted ion chromatogram for the molecular ion. An IDL of 18.7 fg was achieved 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

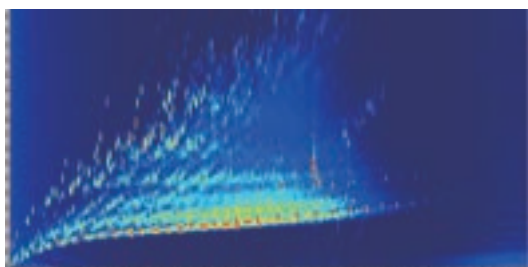
Wide Dynamic Range: 4 orders or more

OFN at concentrations ranging from 0.05 to 1,500 pg/uL (4 orders or more) 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

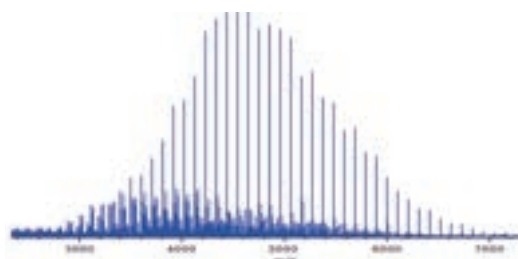
For GCxGC and Fast GC analyses, the chromatographic peaks are very narrow, thus requiring a mass spectrometer that supports high-speed data acquisition. The AccuTOF™ GC-Alpha is a good match for these advanced chromatographic techniques because it can acquire data at up to 50 spectra per second.



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.

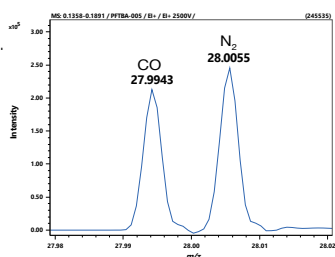


FD mass spectrum of polystyrene 5200

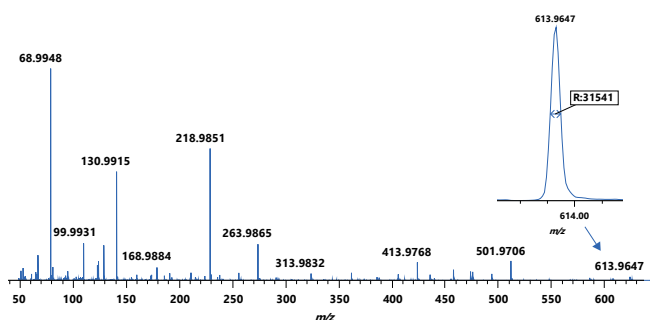
High Mass Resolving Power: 30,000

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



Mass separation of m/z 28



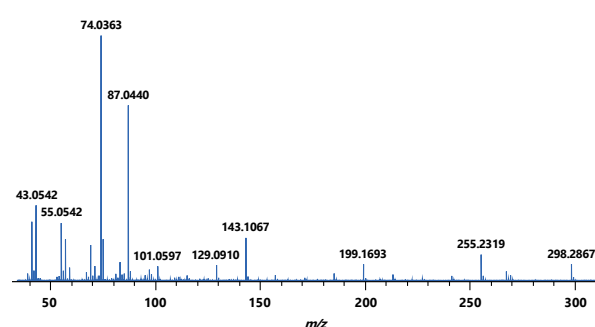
EI mass spectrum of PFTBA

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 ₁₂ 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 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 AccuTOF™ 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).

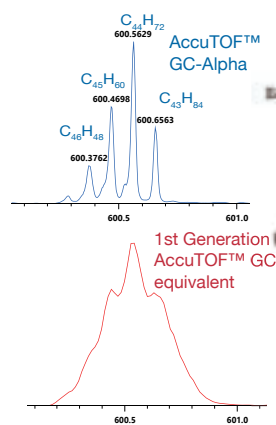


Benefits of High Mass Accuracy

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.

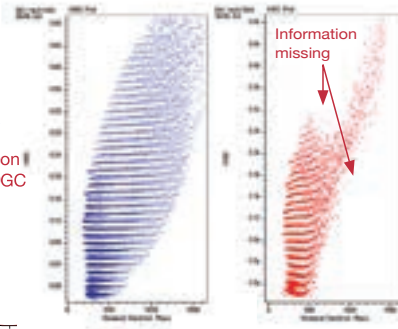
The higher mass accuracy of the AccuTOF™ GC-Alpha makes it possible to use a smaller mass tolerance which in turn reduces the number of candidate elemental compositions. As a result, the user can more easily determine the correct compositions!

FD Mass Spectrum of Crude Oil



KMD Plot of Crude Oil

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



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 ₃	3.0	638.54799	1.41	100
3	C ₃₈ H ₈₀ N ₁₀	9.0	638.54664	2.76	100
4	C ₂₉ H ₇₀ N ₁₆ 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 ₃	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

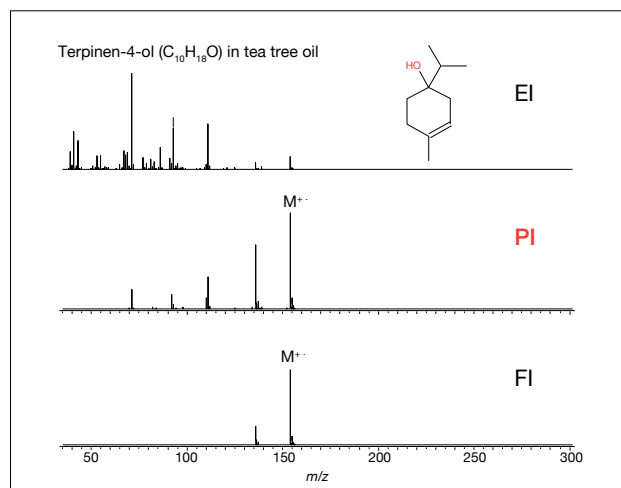


Soft ionization - a powerful tool for qualitative analysis

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.



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)

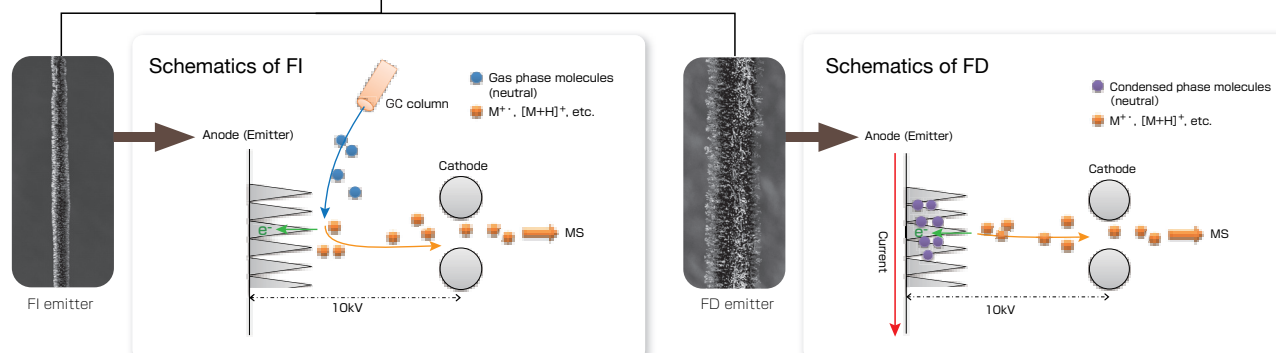
- ▶ The sample is introduced to the ion source through GC or a standard sample inlet system.
- ▶ Unlike CI, FI uses no reagent gas; no need to choose a reagent gas appropriate for the analyte.

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.

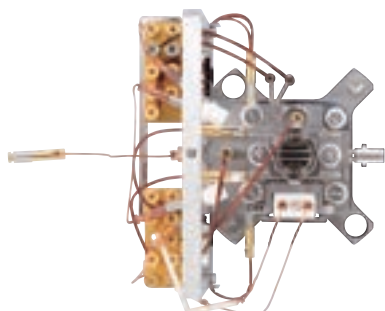


Probe tip for the emitter



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 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)



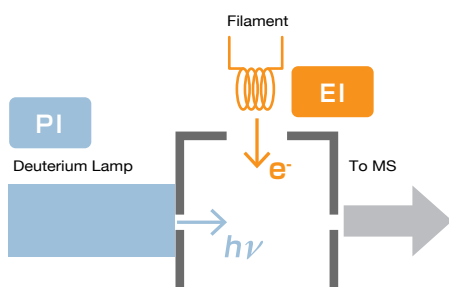
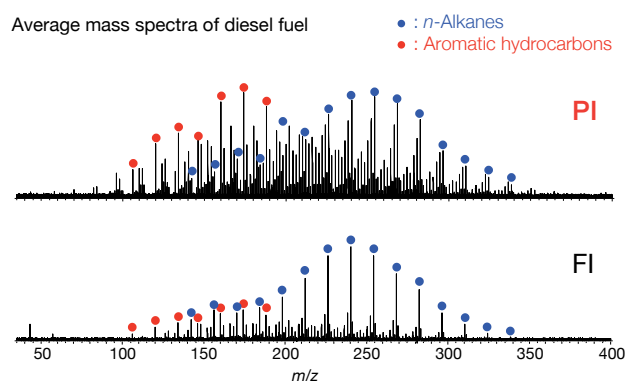
EI/PI

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 vacuum
- ▶ No need for reagent gases

Average mass spectra of diesel fuel



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

Schematics of EI/PI Combination Ion Source

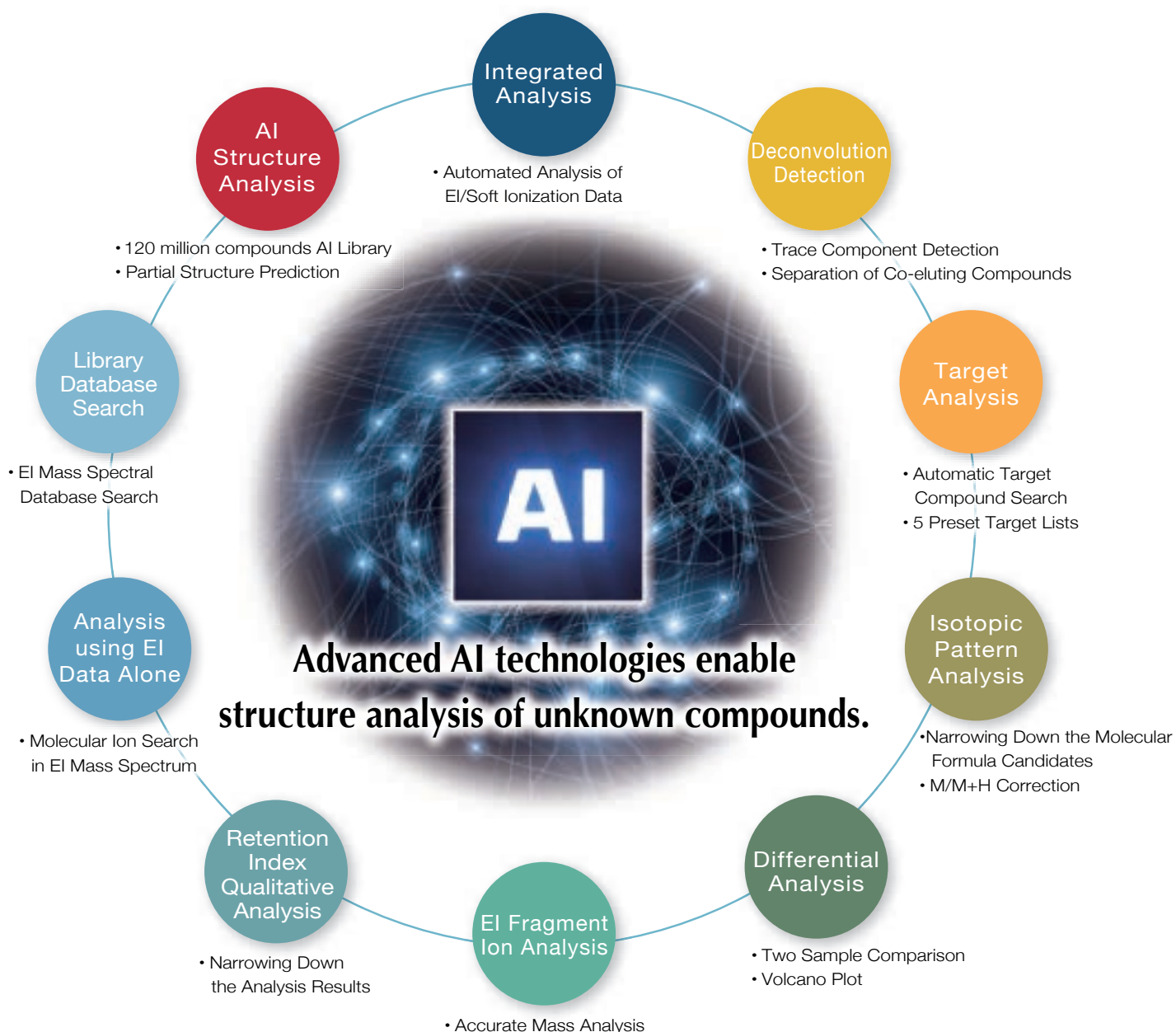
PI is particularly useful for the analysis of aromatic compounds in complex mixtures. These compounds produce high intensity peaks with PI because they strongly absorb UV light.

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



CI

CI is a classical 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.



A new generation of analysis software for simple, speedy operation

msFineAnalysis AI offers a new structure analysis tool for unknowns that is specifically designed for the JEOL JMS-T2000GC "AccuTOF™ GC-Alpha." This next generation software adds this structure analysis capability to improve the overall automatic qualitative analysis functionality that was already available with our previous generation msFineAnalysis. The new "integrated analysis" combines GC/EI high resolution data, GC/soft ionization high resolution data, and "structure analysis" using three AIs (Main AI, Support AI, Prediction of RI). These advanced AI technologies allow msFineAnalysis AI to provide a unique automatic structure analysis capability that was not previously available for GC-MS qualitative analysis.

● ● ● Three Features of AI Structural Analysis



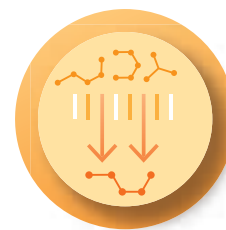
Latest AI Models

- Graph Convolutional Networks
- Prediction of EI mass spectra
- Similarity (average): 0.8
- Accuracy #1 (1st): 41%
- Accuracy #2 (top 1%): 80%



AI Library

- Predicted EI mass spectral library
- New AI Library for 120 million compounds
- Two *in-silico* libraries for specific applications:
 - Pyrolyzates: 10 million compounds
 - TMS derivatives: 5 million compounds



Structure Filtering

- Prediction of retention index (RI) from structural formula
- Narrow down candidate structural formulas by comparing measured and predicted RI values
- Filtering by substructure

※ AI models are not included in the product. AI library created with the latest AI models and structural formula filtering functions are included.

Unknown Compounds Identification and Known Compounds Quick Search Widely applicable for GC-MS qualitative analysis in various markets and fields!



Polymers and Materials

- Unknown compound analysis by pyrolyzates AI library
- Differential analysis
- Target analysis for additives



Food

- Retention Index Qualitative Analysis
- Target analysis for PAHs
- Unknown compound analysis in food



Aroma and Fragrance

- Target analysis for off-flavors
- Unknown flavor analysis
- Trace compound detection by deconvolution function



Petroleum

- Unknown compound analysis in petroleum
- Target analysis of additives in pyro-oil



Environmental

- Unknown compound analysis in environment
- Target analysis of VOCs and organic pollutants in the atmosphere



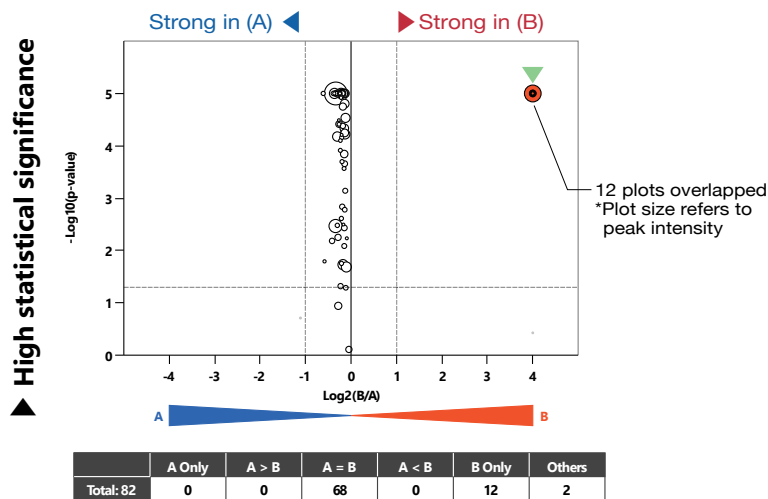
Metabolomics

- Unknown compound analysis by TMS derivatives AI library
- Differential analysis

Qualitative Analysis Application

for non-target analysis and target analysis

Structural analysis of contaminants in a polypropylene product (MSTips No.424)



Differential analysis and volcano plot analysis are effective in examining the difference between two samples, such as normal and defective samples. In this case, we found 12 characteristic components in the PP defective samples.

Nine of these 12 components were unknown compounds not registered in the NIST library. AI structural analysis of these 9 compounds revealed that all of the structures were suggestive of mixed dimers and trimers of acrylonitrile-styrene (AS) copolymer, and were consistent with the literature with high accuracy¹⁾.

It was possible to identify that the contaminant mixed in the defective product (B) was the AS copolymer.

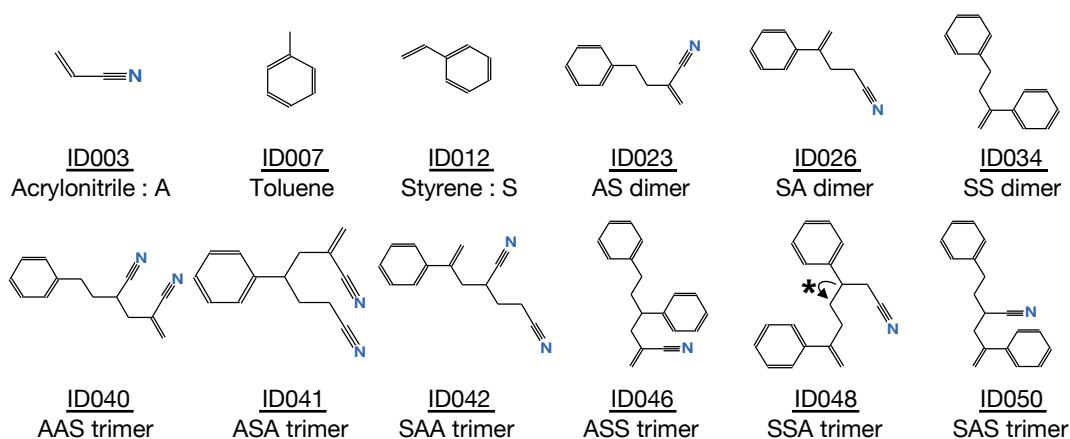
Volcano plot for normal product (A) and defective product (B)

1) Shin Tsuge, Hajime Ohtani, Chuichi Watanabe (2011), Pyrolysis - GC/MS Data Book of Synthetic Polymers, Elsevier

ID	General				Compound Name	Lib.	Total Result						
	RT [min]	Height [%]	IM m/z				Similarity / AI Score	Formula	DBE	Calculated m/z	Mass Error [mDa]	Isotope Matching	El Fragment Coverage
003	1.27	4.83	53.02651		2-Propenenitrile	mainlib	778	C3 H3 N	3.0	53.02600	0.51	0.91	100
007	3.00	2.15	92.06214		Toluene	mainlib	921	C7 H8	4.0	92.06205	0.09	0.89	100
012	5.09	65.31	104.06269		Styrene	mainlib	965	C8 H8	5.0	104.06205	0.64	0.96	100
023	12.14	4.99	157.08970		2-methylidene-4-phenylbutanenitrile	AI	904	C11 H11 N	7.0	157.08860	1.09	0.94	100
026	13.25	3.54	157.08966		4-phenylpent-4-enenitrile	AI	855	C11 H11 N	7.0	157.08860	1.06	0.91	100
034	16.86	2.90	208.12615		3-phenylbut-3-enylbenzene	AI	833	C16 H16	9.0	208.12465	1.50	0.86	100
040	17.68	2.80	210.11566		2-methylidene-4-(2-phenylethyl)pentanedinitrile	AI	729	C14 H14 N2	9.0	210.11515	0.51	0.67	100
041	17.98	8.52	210.11544		2-methylidene-4-phenylheptanedinitrile	AI	622	C14 H14 N2	9.0	210.11515	0.29	0.69	100
042	18.26	3.28	210.11623		2-(2-phenylprop-2-enyl)pentanedinitrile	AI	711	C14 H14 N2	9.0	210.11515	1.08	0.88	92
046	20.70	3.63	261.15184		2-methylidene-4,6-diphenylhexanenitrile	AI	660	C19 H19 N	11.0	261.15120	0.64	0.72	100
048	21.09	3.93	261.15180		3,6-diphenylhept-6-enenitrile	AI	538	C19 H19 N	11.0	261.15120	0.60	0.80	100
050	21.33	9.43	261.15152		4-phenyl-2-(2-phenylethyl)pent-4-enenitrile	AI	597	C19 H19 N	11.0	261.15120	0.32	0.85	100

mainlib=NIST library, AI=AI structure analysis

Qualitative analysis results of 12 components specific to the defective product (B)



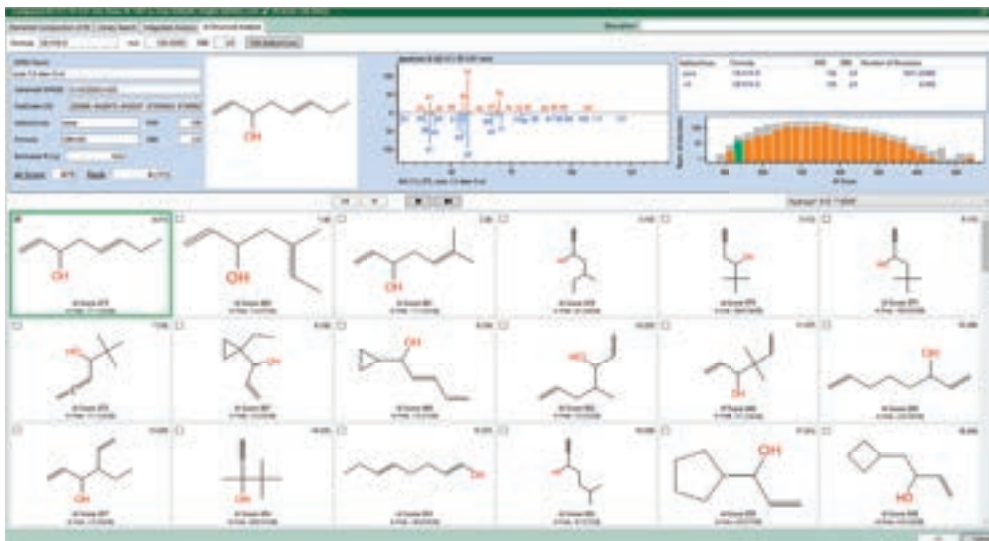
* Side chain position differs from literature

Estimated structure formula of 12 specific compounds in the defective product (B)

Structural analysis of unknown compounds in foods

We carried out an analysis of flavor components in oysters as an analysis of unknown substances in foods. AI structure analysis of the component, which had been identified as 1,5-Octadien-3-ol in the paper²⁾, yielded 2,560 candidate structural formulas, which were narrowed down to 1,031 candidates using the "OH" substructure filter. The structural formula proposed by the paper was the 4th hit with a higher scoring of 875.

2) Kenji Ueda, Koki Yahiro, Yoshihiko Akakabe, J. Oleo Sci. 72, (7) 725-732 (2023)



AI structural analysis result window of the flavor component in oyster



JMS-T2000GC with a HS-SPME (headspace – solid phase microextraction) autosampler

Target analysis of flavor and off-flavor components in foods

msFineAnalysis AI supports not only non-target analysis but also target analysis. It automatically searches for target compounds based on compositional formula, m/z value and CAS#.

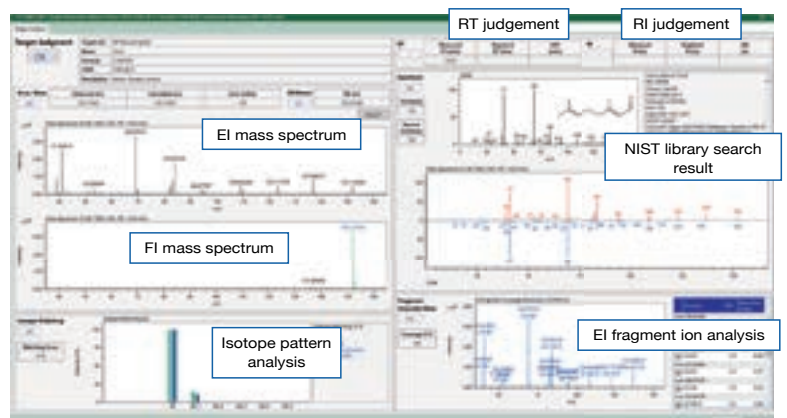
For the data of flavor components in lemon juice, 10 compounds were extracted when searching an off-flavor list that targeted 498 different compounds. The result window on the lower right shows the detailed analysis result of Citral among the 10 compounds.

The screenshot shows a table with multiple columns containing chemical names, molecular weights, and other identifiers for 498 off-flavor components. The text is small and dense, typical of a data-rich software interface.

Target list of 498 components of off-flavor (preset list)

Preset target lists

- ▶ Off-flavors: 498 compounds
- ▶ Additives: 409 compounds
- ▶ VOCs: 222 compounds
- ▶ Organic air pollutants: 224 compounds
- ▶ PAHs: 28 compounds

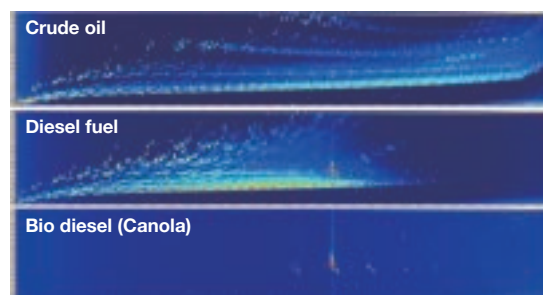
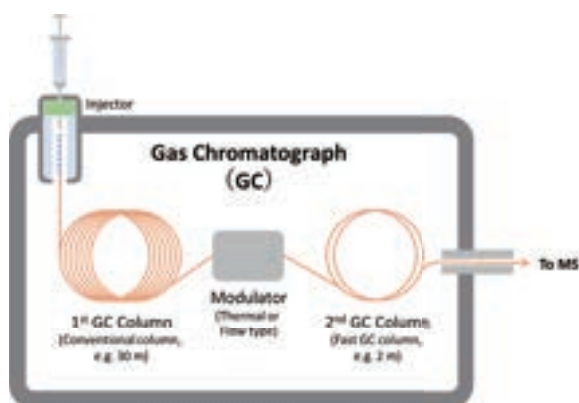
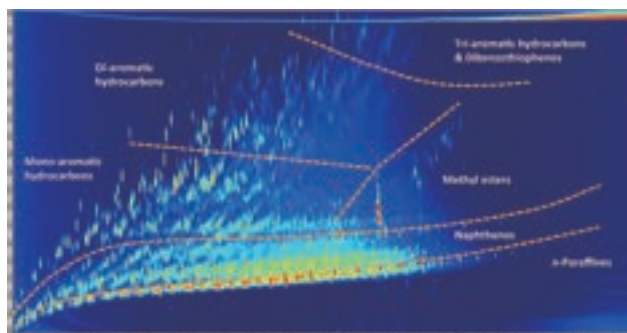


Detailed analysis of Citral present in lemon juice

AccuTOF™ GC-Alpha with comprehensive 2D GC (GCxGC)

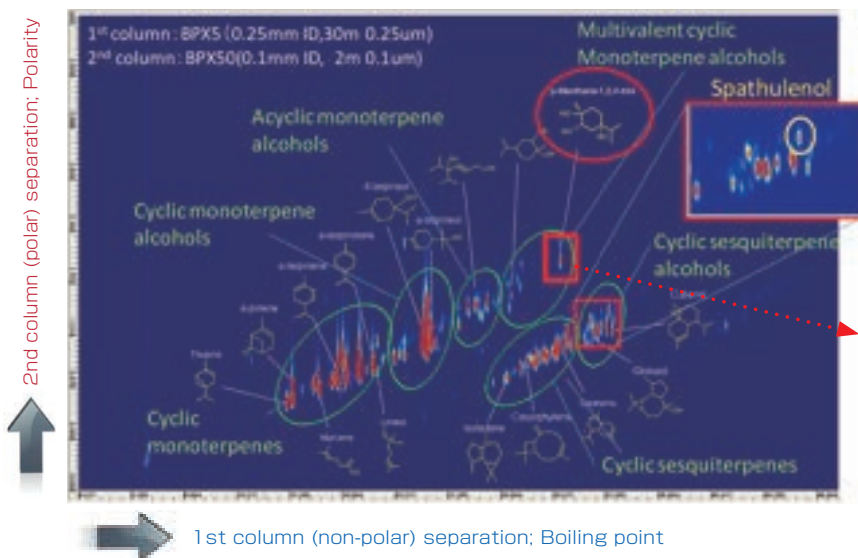
GCxGC is an ultrahigh-separation chromatography system that uses 2 GC columns with different polarities in series. The eluted components from the 1st column are trapped and then released at specified intervals into the 2nd column using a modulator between the two columns. High-speed data acquisition 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.

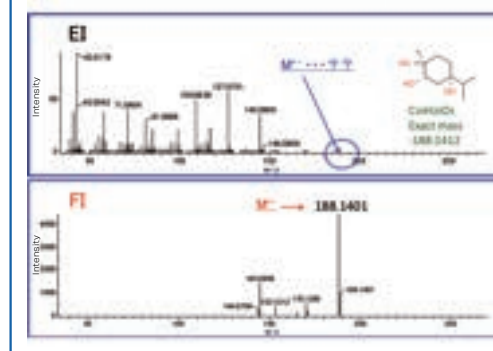


GCxGC-TOFMS Analysis of Tea Tree Oil (MSTips No.233)

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 TIC of tea tree oil by GCxGC/TOFMS

* For measurement, ZOE's GCxGC system was used. GCxGC chromatogram was created by GC Image, LLC's GC Image software.

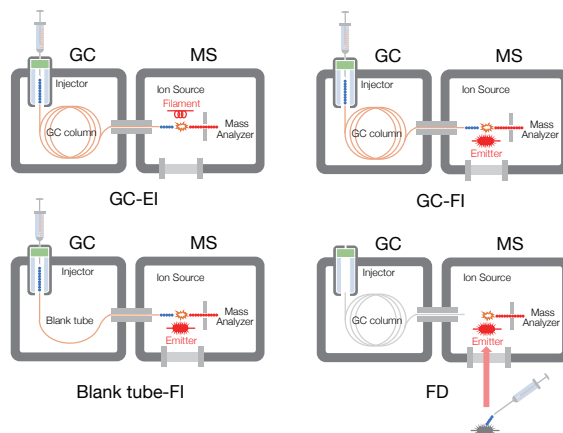
AccuTOF™ GC-Alpha for petroleum

The FI/FD method is an effective method as soft ionization of hydrocarbon compounds that are often present in petroleum samples. The AccuTOF GC-Alpha is capable of petroleum analysis by three measurement methods.

Comparison of the three measurement methods

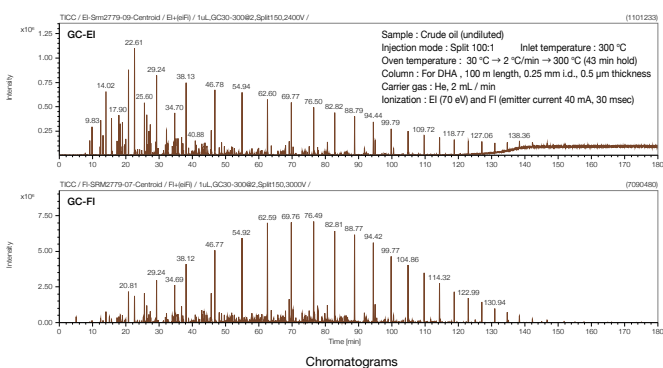
These measurement methods can be used depending on the boiling point range of the sample and the purpose of the analysis. EI/FI/FD combination ion sources can be used for all types of measurements.

Method	Separation	Low-boiling (b.p. < 200 °C)	High-boiling (b.p. up to 550 °C)	Very high-boiling (b.p. > 550 °C)	Meas. Time
GC/FI	GC + MS	Excellent	Fair	Not suitable	Long (~30 min.)
Blank Tube FI	MS only	Excellent	Good	Fair	Very quick (~1 min.)
FD	MS only	Not suitable	Excellent	Good	Very quick (~1 min.)

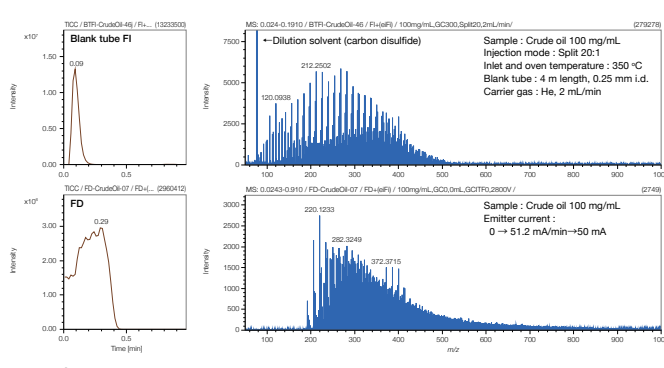


Crude oil analysis

GC/EI and FI methods are suitable for low boiling point components and isomer analysis. The FD method is suitable for type analysis targeting high-boiling components, and the blank tube FI method is suitable for comprehensive analysis of low to high-boiling components.



GC/MS measurement data
Upper: GC/EI, Lower: GC/FI



Direct MS measurement data
Upper: Blank Tube FI, Lower: FD



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.

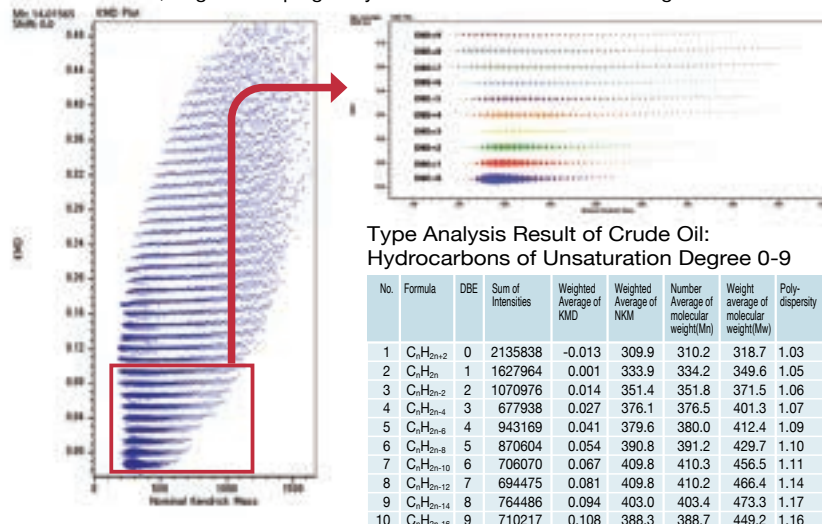
Moreover, by grouping each series, a type analysis calculation can automatically be performed for each group that includes:

- ▶ 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 _n H _{2n+2}	0	2135838	-0.013	309.9	310.2	318.7	1.03
2	C _n H _{2n}	1	1627964	0.001	333.9	334.2	349.6	1.05
3	C _n H _{2n-2}	2	1070976	0.014	351.4	351.8	371.5	1.06
4	C _n H _{2n-4}	3	677938	0.027	376.1	376.5	401.3	1.07
5	C _n H _{2n-6}	4	943169	0.041	379.6	380.0	412.4	1.09
6	C _n H _{2n-8}	5	870604	0.054	390.8	391.2	429.7	1.10
7	C _n H _{2n-10}	6	706070	0.067	409.8	410.3	456.5	1.11
8	C _n H _{2n-12}	7	694475	0.081	409.8	410.2	466.4	1.14
9	C _n H _{2n-14}	8	764486	0.094	403.0	403.4	473.3	1.17
10	C _n H _{2n-16}	9	710217	0.108	388.3	388.7	449.2	1.16

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

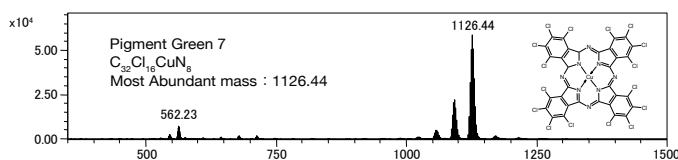
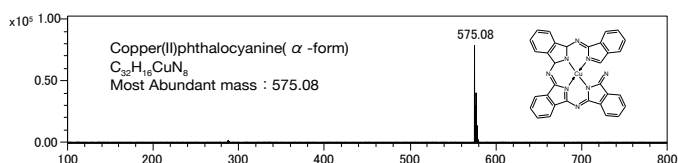
- ▶ Sample dissolved or dispersed in solvent is applied to the carbon emitter at the tip
- ▶ Suitable for high boiling point, high molecular weight, and/or thermally labile compounds
- ▶ Suitable for low- to mid-polar metal complexes
- ▶ Used for FD soft ionization



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.



FD mass spectra of pigments

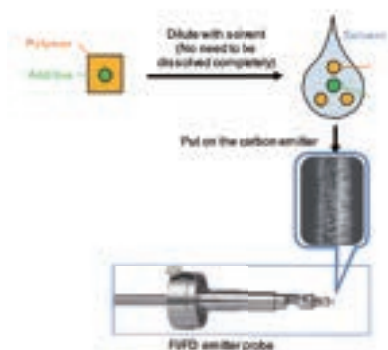
FD Sampling Tool

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



FD Sampling Tool

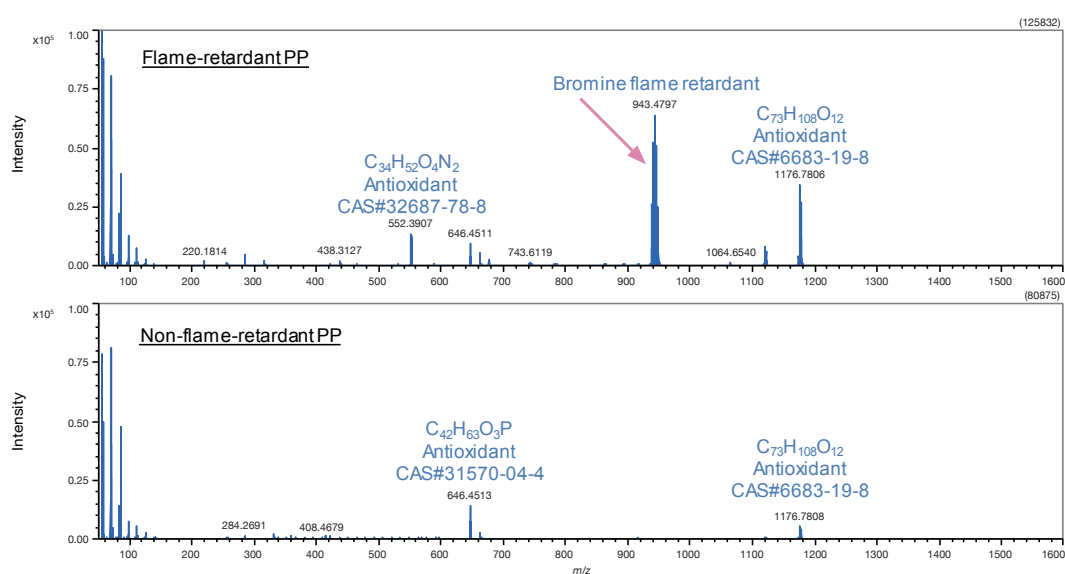
Analysis of brominated flame retardants in polypropylene products by FD (MSTips No.355)



In the FD method, the sample is dissolved or dispersed with a solvent and then applied onto the emitter to be introduced into the ion source. The sample does not need to be completely dissolved in the solvent.

In this case, it is possible to analyze only the additives in the solvent. Since it is a direct sample injection method without using a column, high boiling point (high mass) components can be measured. Since it is soft ionization, molecular ions can be detected.

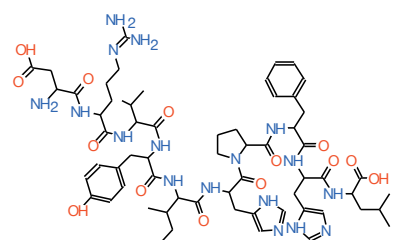
A clear difference peak was detected at m/z 943.4797 from the flame-retardant PP. It was estimated to be a brominated flame retardant by isotope pattern analysis and composition estimation.



FD mass spectra, Upper: Flame-retardant PP, Lower: Non-flame retardant PP

Peptide measurement by FD method (MSTips No.445)

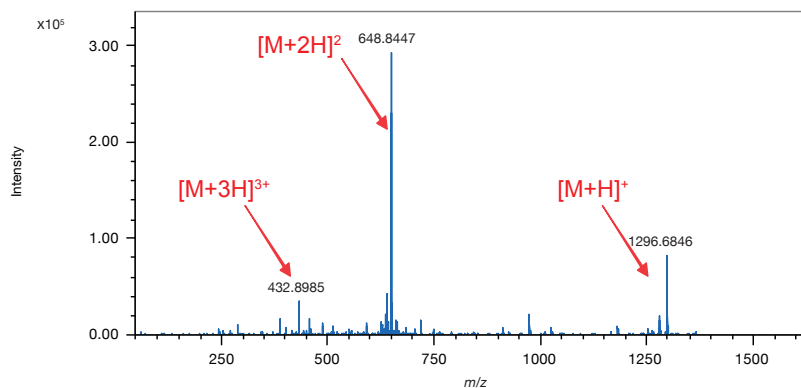
Highly polar compounds that are difficult to measure by GC-MS can also be analyzed by the FD method. Composition formula calculation by accurate mass measurement is also available.



Asp-Arg-Val-Tyr-Ile-His-Pro-Phe-His-Leu

Formula: $C_{62}H_{89}N_{17}O_{14}$

Structural formula of Angiotensin I

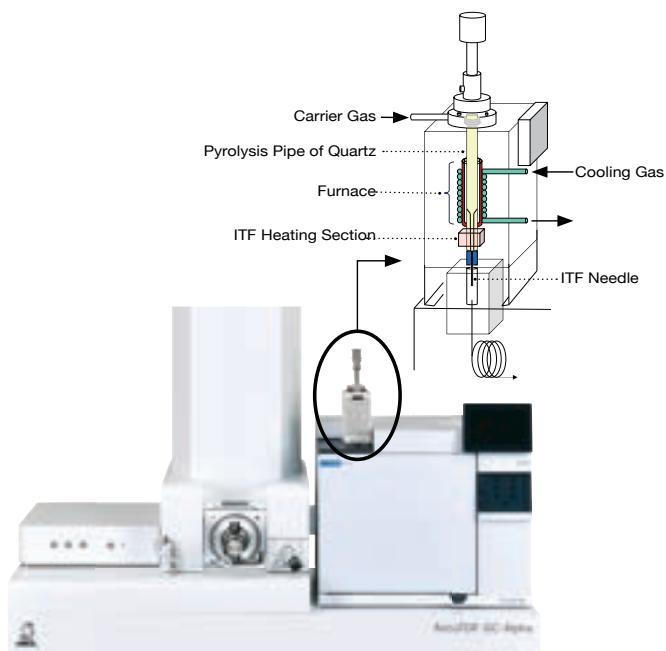


Ion Type	Measured m/z	Formula	Calculated m/z	Mass Error [mDa]
$[M+H]^+$	1296.68462	$C_{62}H_{90}N_{17}O_{14}$	1296.68477	-0.15
$[M+2H]^{2+}$	648.84471	$C_{62}H_{91}N_{17}O_{14}$	648.84602	-1.31
$[M+3H]^{3+}$	432.89845	$C_{62}H_{92}N_{17}O_{14}$	432.89977	-1.32

FD mass spectrum and accurate mass analysis for Angiotensin I

Pretreatment hardware options that meet your needs

Pyrolysis (Py)



■ Pyrolyzer

A pyrolyzer system is capable of thermal extraction and/or pyrolysis and is mainly used for measuring solid samples such as polymeric materials. The photo shows the combination with the Multi-Shot Pyrolyzer (EGAPY-3030D) manufactured by Frontier Laboratories Ltd.

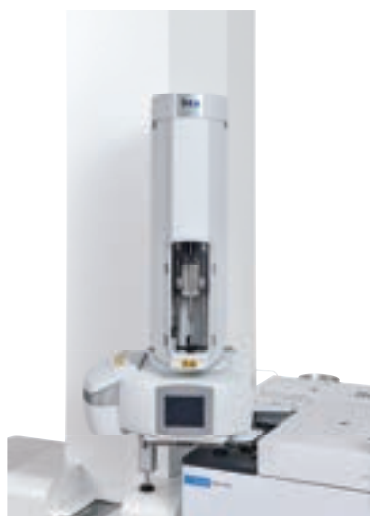
Thermogravimetry/Differential Thermal Analysis (TG/DTA)



■ TG/DTA

TG-DTA is a device to evaluate thermophysical properties such as exothermal and endothermal properties associated with weight change and chemical change during the heating process of a solid sample. By connecting with MS, components generated in the heating process can be analyzed in real time. The photo shows the combination with the STA449 manufactured by NETZSCH.

Multi-function Autosampler



■ Multi-function Autosampler

These systems can perform various measurements such as liquid injection, headspace (HS), and solid-phase microextraction (SPME). The photo shows the combination with 2850T by HTA and combi PAL system by CTC Analytics.

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)

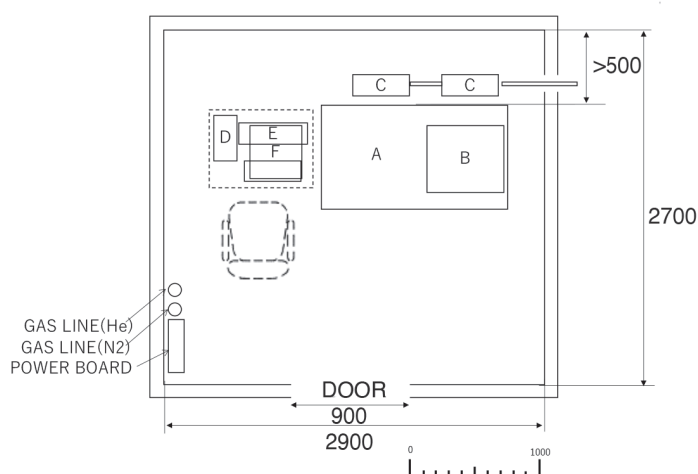
Power supply requirement depends on a specific configuration sold in each territory. Please inquire at a local sales office for details.

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) $25 \mu\text{m}$ or less Accelerating Voltage 0.1 m/s^2 or less
Room Temperature	20 to 27 °C
Temperature fluctuation	± 3 °C/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



< 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.

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.

Windows is a registered trademark or trademark of Microsoft Corporation in the U.S.A. and other countries.

* Appearance and specifications are subjected to change without notice.

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3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3561 Fax. +81-3-6262-3577
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▼ Local office



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