Scientific / Metrology Instruments

Gas Chromatograph — Time-of-Flight Mass Spectrometer

Solutions for Innovation

JMS-T2000GC

AccuTOF™ GC-Alpha 2.0

Pursuing the ultimate in performance
and functionality

JEOL Ltd.

AccuTOF™ GC-Alpha 2.0

The ultimate GC-MS system that pursues the ultimate in performance and functionality, the JMS-T2000GC AccuTOF™ GC-Alpha, has evolved into version “2.0” with the integration of a fully automated standard sample inlet and msFineAnalysis AI. It enables automatic structural analysis of unknown compounds from comprehensive two-dimensional gas chromatography (GCxGC) data, revolutionizing the conventional approach to qualitative analysis using GC-MS.

JMS-T2000GC AccuTOF™ GC-Alpha 2.0

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/FD 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

2020

JMS-T2000GC AccuTOF™ GC-Alpha

- New ion optics
- Vast improvement of mass resolving power (10,000 → 30,000)
- Vast improvement of mass accuracy (3 ppm → 1 ppm)

2022

msFineAnalysis AI

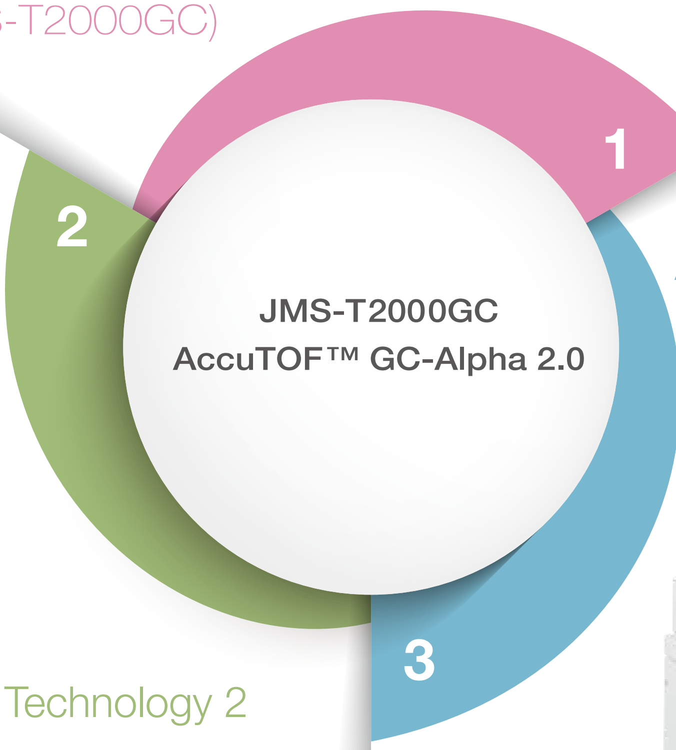
- Automatic structural analysis of unknows with AI technology

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, designed for use with vacuum ion sources that included EI, CI, FI, and FD, was launched. This system was the first GC-TOFMS to provide accurate mass measurements while achieving a mass resolving power of 5,000 and a spectrum recording speed of 25 Hz.

The legacy of the AccuTOF™ series continues to the AccuTOF™ GC-Alpha 2.0 (and beyond).

Aiming for high performance while keeping it simple, the **AccuTOF™ GC-Alpha 2.0** uses three Key Technologies.



Key Technology 1

GC-TOFMS Technology

(JMS-T2000GC)

Key Technology 2

Soft Ionization Technology

(EI/FI, EI/PI, CI)

Key Technology 3

AI Structural Analysis Technology

(msFineAnalysis AI)

Key Technology 1

High-performance Time-of-Flight Mass Spectrometer

The AccuTOF™ GC-Alpha 2.0 is the 7th generation JEOL GC-TOFMS since the original AccuTOF™ GC.

The AccuTOF™ GC-Alpha 2.0 employs orthogonal-acceleration time-of-flight mass spectrometer (oaTOFMS) with dual stage reflectron, an ideal ion optical system realizing both high ion transmission (= sensitivity) and ultra-high mass resolving power.

Key Technology 2

Soft ionization methods: absolutely essential for unknown compound analysis

The following soft ionization methods are available for AccuTOF™ GC-Alpha 2.0

- 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-TOFMS, is a qualitative analysis software with the following features:

1. Structural analysis of unknowns powered by 4 AI models.
2. GCxGC data analysis
3. Target analysis
4. Deconvolution detection
5. Differential analysis

The msFineAnalysis AI is an innovative GC-MS qualitative analysis software that supports both non-targeted and targeted analysis, and proposes chemical structures for unknown compounds.

Basic Performance of AccuTOF™ GC-Alpha 2.0

High performance for both qualitative and quantitative analyses

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

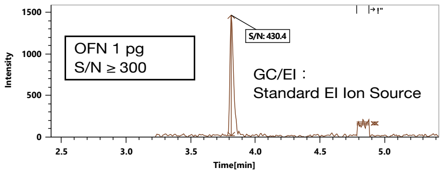
The JMS-T2000GC AccuTOF™ GC-Alpha 2.0 is a high performance GC-MS system that simultaneously realizes high mass resolution, high mass accuracy, high sensitivity, high speed data acquisition, wide dynamic range, and wide mass range.

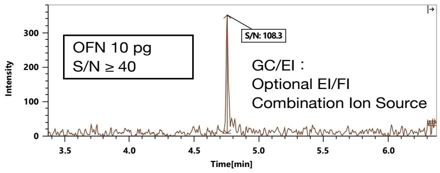
The high mass resolution and high mass accuracy offers unprecedented qualitative analysis results. The high-speed data acquisition can be used for advanced GC-MS measurements such as comprehensive two-dimensional GC (GCxGC), while the wide dynamic range is useful for not only quantitative analysis but 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.

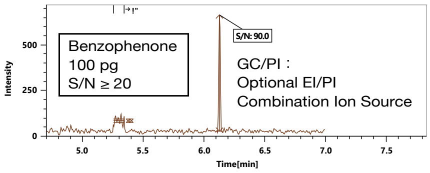
The AccuTOF™ GC-Alpha 2.0 is truly a high performance GC-MS system that removes the limitations for chemical analysis!

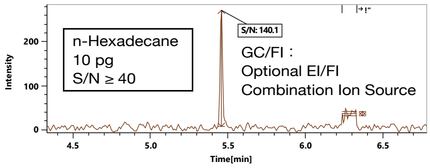
High Sensitivity

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





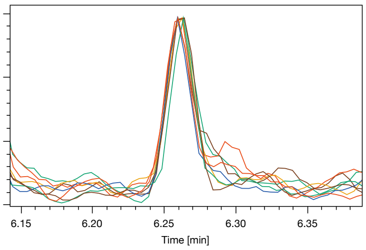




OFN: Octafluoronaphthalene

Instrument Detection Limit: IDL = 18.7 fg

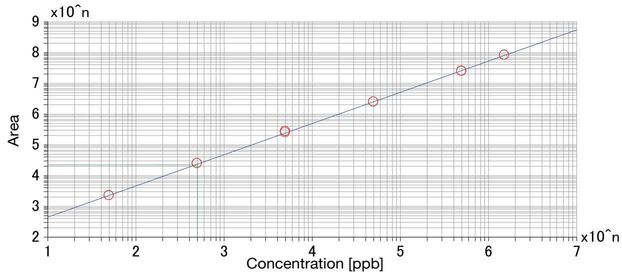
Eight sequential measurements of 100 fg of octafluoronaphthalene (OFN) were obtained by using the standard EI ion source.
The instrument detection limit (IDL) is calculated based on the peak area and reproducibility of the extracted ion chromatogram for the molecular ion. An IDL of 18.7 fg was achieved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

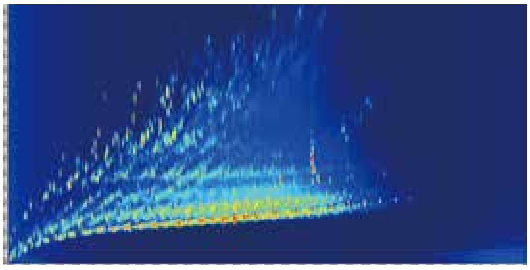
Wide Dynamic Range: 4 orders or more

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

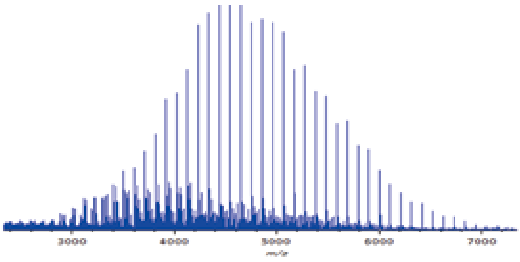
For GCxGC and Fast GC analyses, the chromatographic peaks are very narrow, thus requiring a mass spectrometer that supports high-speed data acquisition. The AccuTOF™ GC-Alpha 2.0 is a good match for these advanced chromatographic techniques because it can acquire data at up to 50 spectra per second.



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* 1,000, while the AccuTOF™ GC-Alpha 2.0 can detect *m/z* 6,000 and higher. This makes it possible to use direct probe MS methods such as field desorption (FD) to measure samples like oligomers.

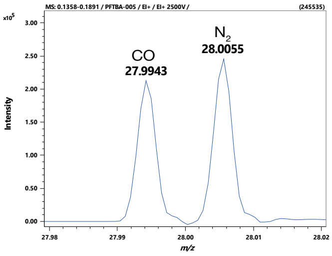


FD mass spectrum of polystyrene 5200

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 following advantages:

- Separation and detection of closely spaced *m/z* ions (see right figure)
- Stable centroid position of ion peaks, resulting in improved mass accuracy



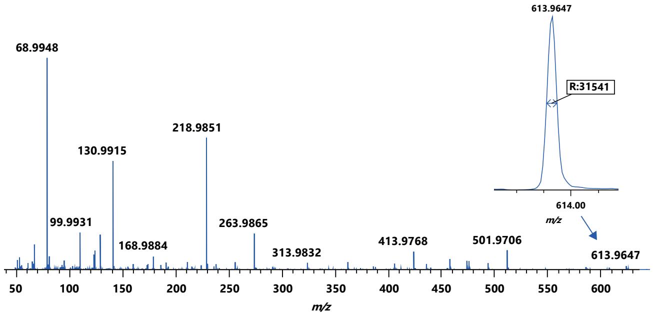
Mass separation of *m/z* 28

High Mass Accuracy: 1 ppm*

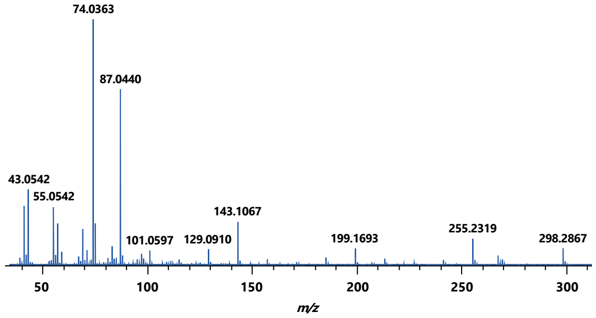
High mass accuracy makes it possible to determine the elemental compositions for the observed ions. Using the "drift compensation - multiple" mass calibration function, the average mass accuracy (absolute value) for 10 ions observed from methyl stearate was 0.05 mDa or 0.45 ppm.

* Based on our standard for testing.

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

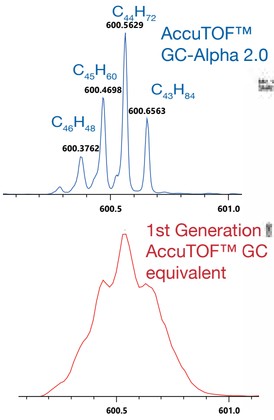
Benefits of
High Mass Resolving Power

When comparing the mass spectra of crude oil from the first generation AccuTOF™ GC and the latest JMS-T2000GC AccuTOF™ GC-Alpha 2.0, each ion is clearly separated and detected with the data obtained using the AccuTOF™ GC-Alpha 2.0.

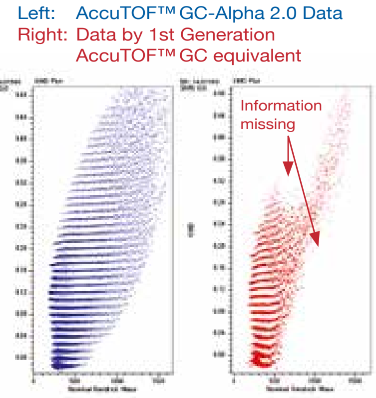
The difference in resolution is clearly evident in the KMD (Kendrick Mass Defect) plot for the FD mass spectrum of crude oil. The lower resolution of the first generation AccuTOF™ GC resulted in poor mass accuracy for unresolved peaks involving isobaric compounds at higher masses.

On the other hand, with the KMD plot drawn for the JMS-T2000GC AccuTOF™ GC-Alpha 2.0, 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



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 2.0 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.

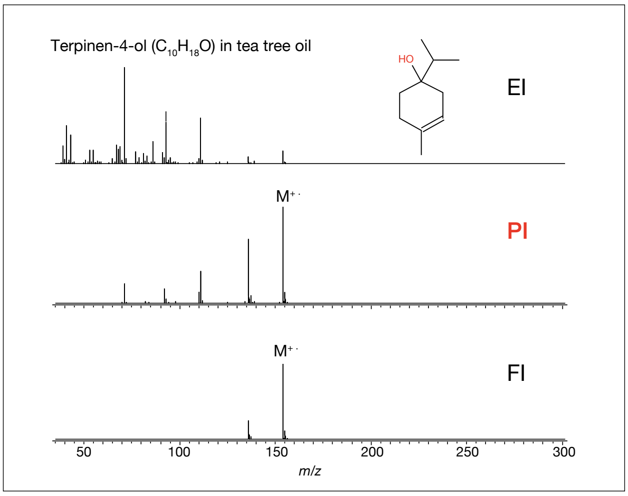
New Qualitative Analysis Capabilities offered by a Variety of Soft Ionizations

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 2.0. 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)

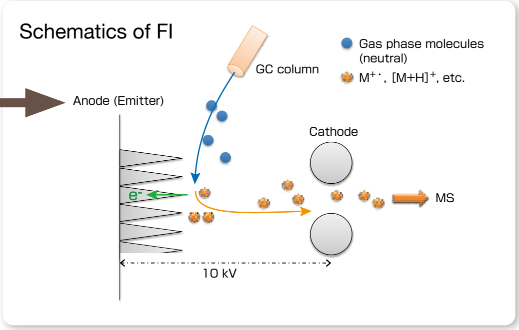
- The sample is introduced to the ion source through GC or a standard sample inlet system.
- Unlike CI, FI uses no reagent gas; no need to choose a reagent gas appropriate for the analyte.

FD (Field Desorption)

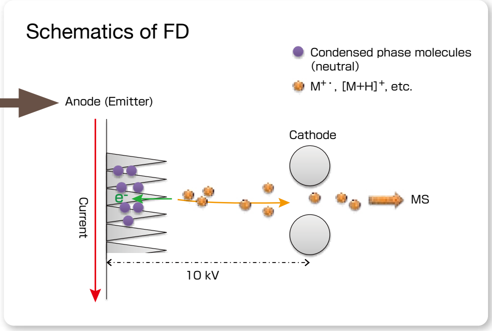
- The sample is applied onto the emitter and directly introduced into the system.
- Suitable for analysis of thermally labile compounds.
- Ideal for samples soluble in nonpolar solvents.
- Analyzes powder samples dispersible in solvents.
- Analyzes low- to mid-polar metal complexes.
- Analyzes high molecular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


Probe tip for the emitter


FI emitter

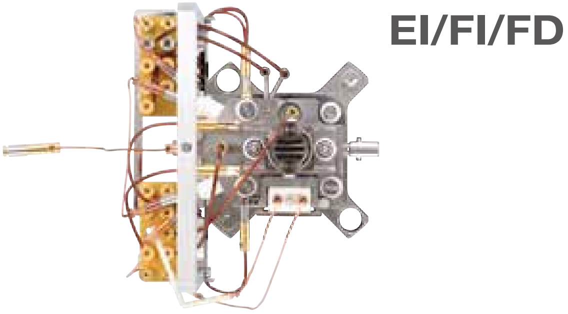

Schematics of FI


FD emitter


Schematics of FD

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)



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.

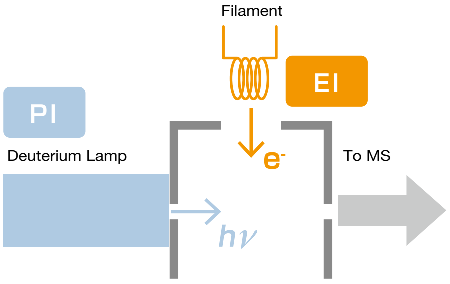
Features

- 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)



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

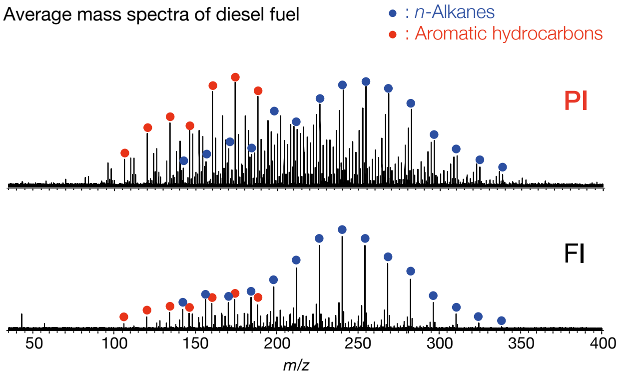
Schematics of EI/PI Combination Ion Source

PI is an ionization method that uses photons from a vacuum ultraviolet (VUV) lamp for ionization. The AccuTOF™ GC-Alpha 2.0 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

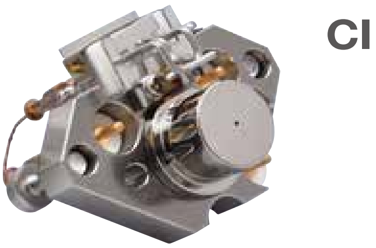
- No need to replace the ion source
- No need to break vacuum
- No need for reagent gases

Average mass spectra of diesel fuel



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 is a classical soft ionization technique that is also optionally available with the AccuTOF™ GC-Alpha 2.0. 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.

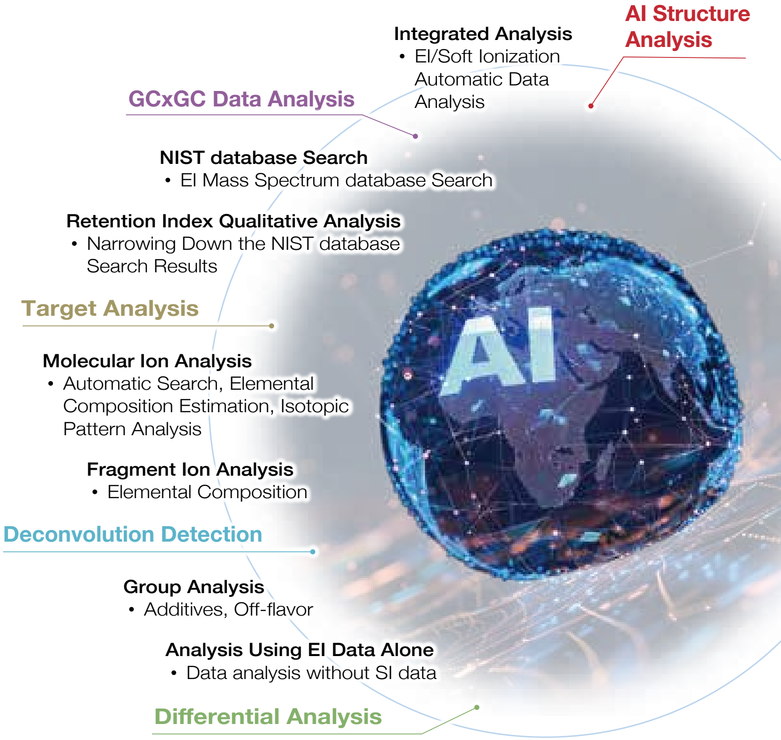
A New Era of Structural Analysis of Unknown Compounds

the Fusion of Cutting-edge AI Technology and Comprehensive GCxGC

msFineAnalysis AI offers a new structure analysis tool for unknown compounds that specifically designed for the JEOL JMS-T2000GC "AccuTOF^{TM} GC-Alpha 2.0". The **"Integrated Analysis"** combines GC/EI, GC/Soft Ionization high resolution data, and the **"AI Structure Analysis"** using four AI technologies.

Version 3 supports comprehensive two-dimensional gas chromatography (GCxGC) data analysis in addition to regular GC-MS data analysis. In complex mixtures such as petroleum samples and life science samples, the ultra-high separation of GCxGC and the structural analysis of unknown compounds using msFineAnalysis AI will prove to be very effective.

These advanced AI technologies allow msFineAnalysis AI to provide a unique automatic structure analysis capability that was not previously available for GC-MS and GCxGC-MS qualitative analysis.



AI Structure Analysis

Integrated Analysis
- EI/Soft Ionization Automatic Data Analysis

GCxGC Data Analysis

NIST database Search
- EI Mass Spectrum database Search

Retention Index Qualitative Analysis
- Narrowing Down the NIST database Search Results

Target Analysis

Molecular Ion Analysis
- Automatic Search, Elemental Composition Estimation, Isotopic Pattern Analysis

Fragment Ion Analysis
- Elemental Composition

Deconvolution Detection

Group Analysis
- Additives, Off-flavor

Analysis Using EI Data Alone
- Data analysis without SI data

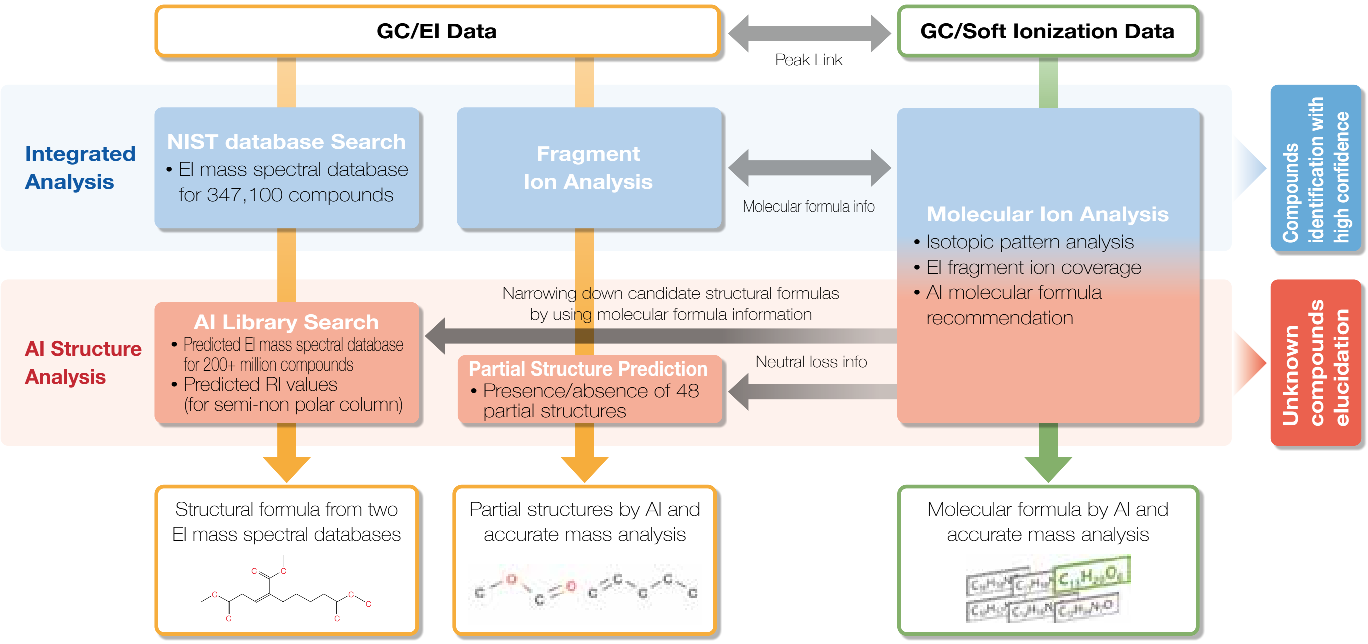
Differential Analysis

Innovative solutions with four AI technologies - Support molecular formula determination and structural formula estimation for unknown compounds

The msFineAnalysis AI utilizes four different AI models to automatically perform analyses on molecular formulas, substructures, and technical know-how, and provides analytical results quickly.

#	Prediction	Software function
1	EI mass spectrum	AI Library
2	Retention Index	AI Library
3	Partial structure	Present or absent for 48 partial structures
4	Molecular formula	AI molecular formula recommendation

Workflow for structural analysis of unknown compounds by msFineAnalysis AI



GC/EI Data

Peak Link

GC/Soft Ionization Data

Integrated Analysis

NIST database Search
- EI mass spectral database for 347,100 compounds

Fragment Ion Analysis

Molecular formula info

Molecular Ion Analysis
- Isotopic pattern analysis
- EI fragment ion coverage
- AI molecular formula recommendation

Compounds identification with high confidence

AI Structure Analysis

AI Library Search
- Predicted EI mass spectral database for 200+ million compounds
- Predicted RI values (for semi-non polar column)

Narrowing down candidate structural formulas by using molecular formula information

Partial Structure Prediction
- Presence/absence of 48 partial structures

Neutral loss info

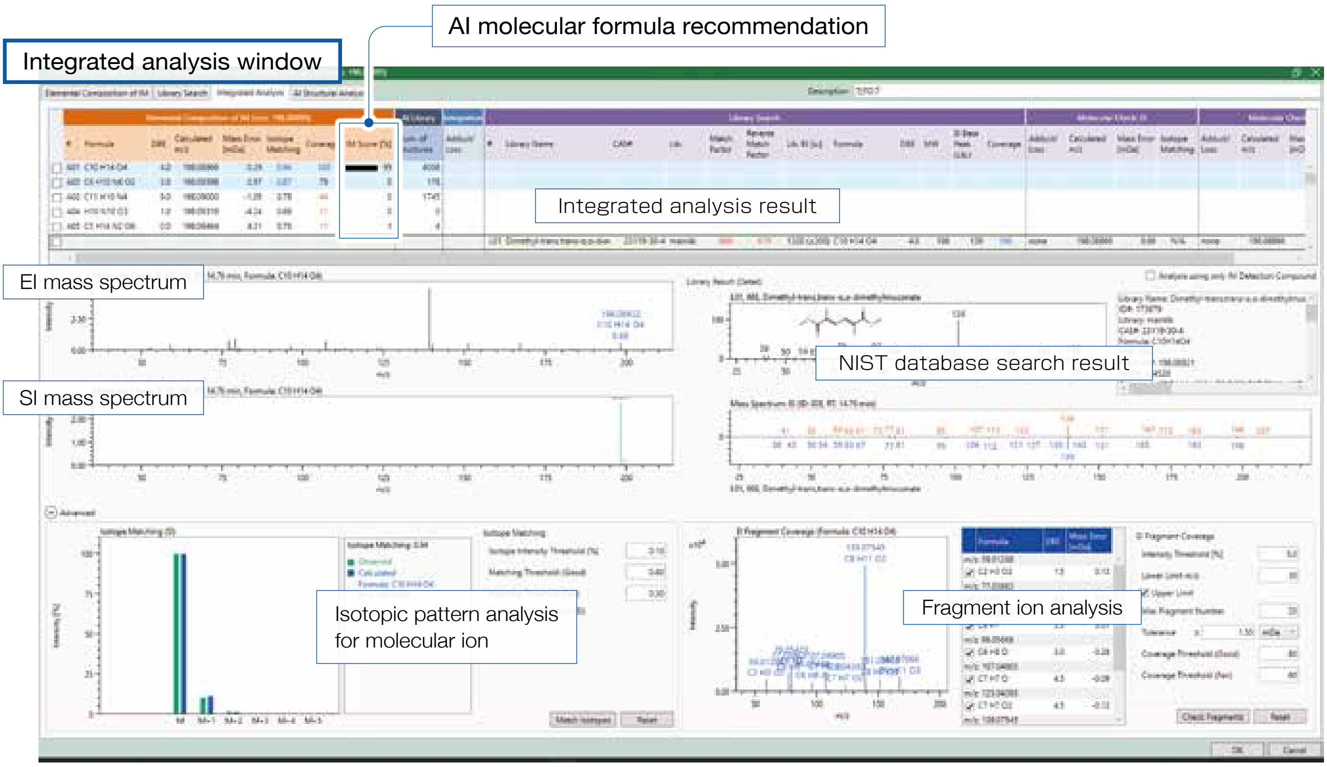
Unknown compounds elucidation

Structural formula from two EI mass spectral databases

Partial structures by AI and accurate mass analysis

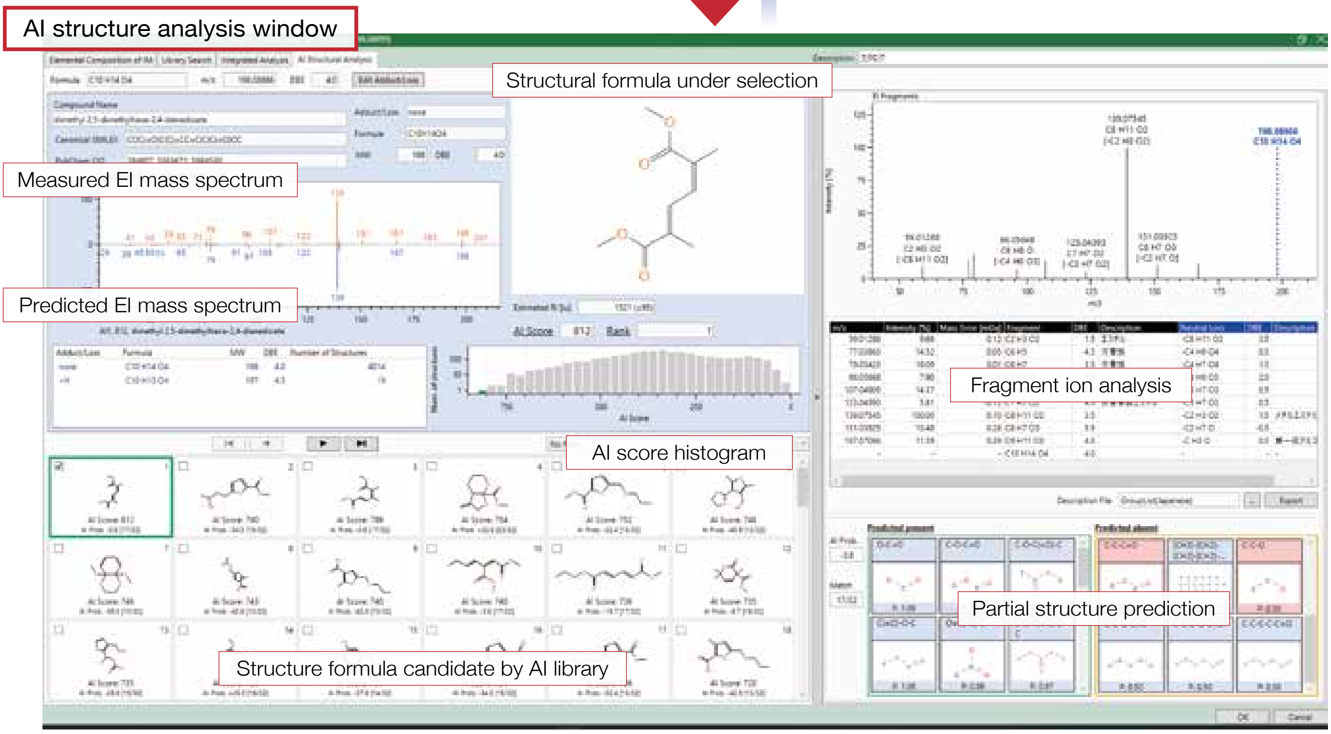
Molecular formula by AI and accurate mass analysis

Compound identification by Integrated Analysis with high confidence



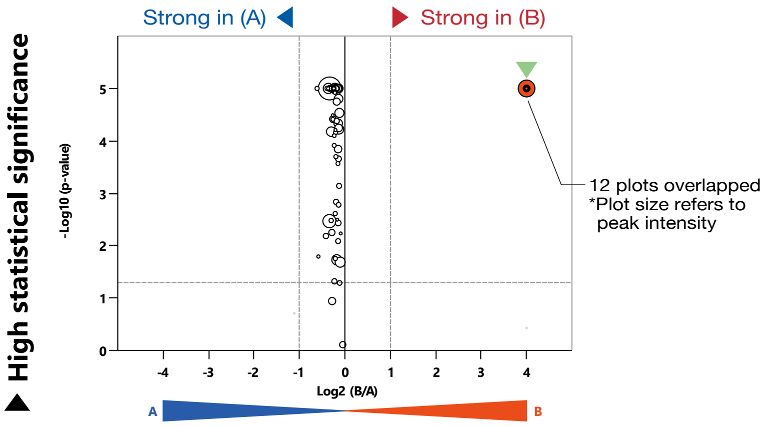
Unknown compound elucidation by AI Structure Analysis

Instantly switch between integrated analysis results and AI structural analysis results by selecting tabs



Qualitative Analysis Application
for non-target analysis and target analysis

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



	A Only	A > B	A = B	A < B	B Only	Others
Total: 82	0	0	68	0	12	2

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

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 accuracy[1).

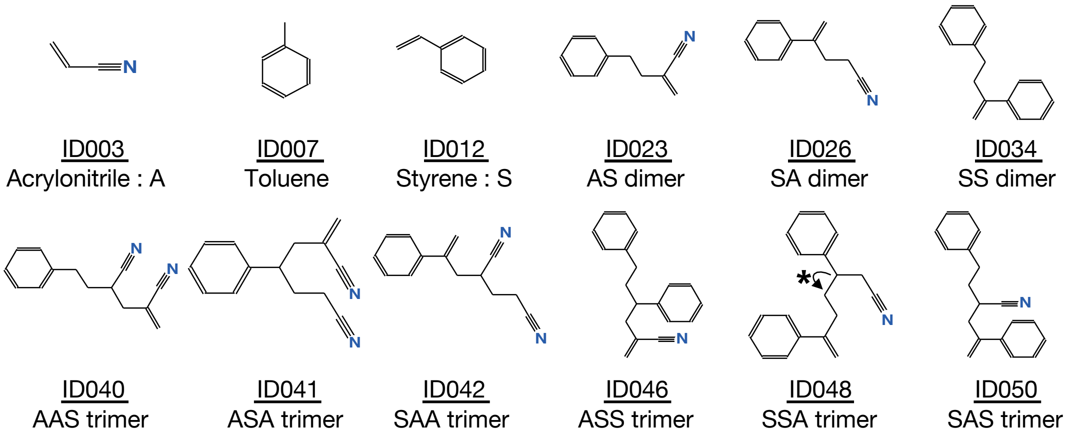
It was possible to identify that the contaminant mixed in the defective product (B) was the AS copolymer.

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

General				Total Result									
ID	RT [min]	Height [%]	IM *m/z*	Compound Name	Lib.	Similarity / AI Score	Formula	DBE	Calculated *m/z*	Mass Error [mDa]	Isotope Matching	EI 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)



ID003 Acrylonitrile : A
ID007 Toluene
ID012 Styrene : S
ID023 AS dimer
ID026 SA dimer
ID034 SS dimer
ID040 AAS trimer
ID041 ASA trimer
ID042 SAA trimer
ID046 ASS trimer
ID048 SSA trimer
ID050 SAS trimer

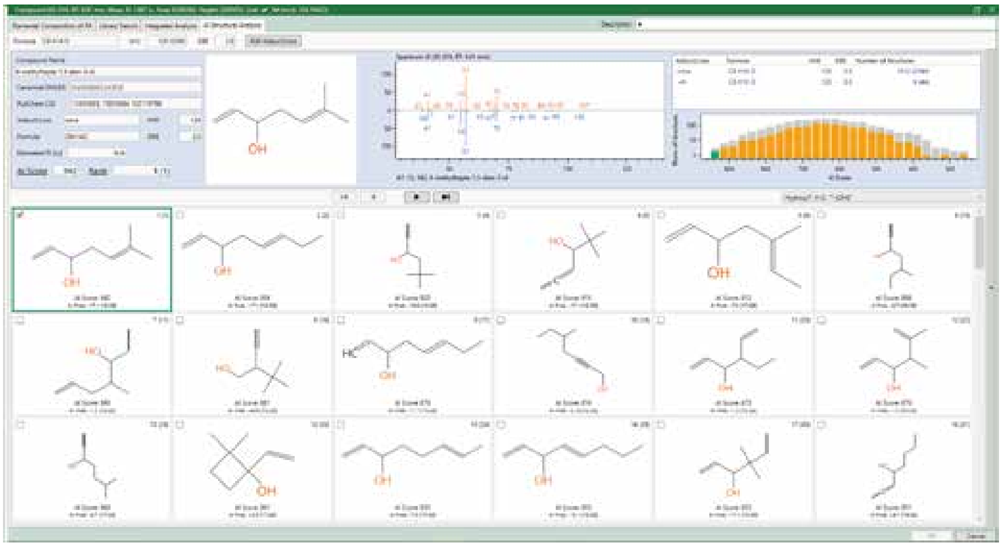
* Side chain position differs from literature

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

Structural analysis of unknown compounds in foods

Flavor components in oysters were analyzed using a combination of HS-SPME GC-MS. AI structure analysis of unknown compounds that was previously identified as 1,5-octadien-3-ol1), yielded 2,544 candidate structural formulas, which were narrowed down to 1,012 candidates using the "OH" substructure filter. The structural formula proposed by the paper was the second hit with an AI score of 936, which is quite high.

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



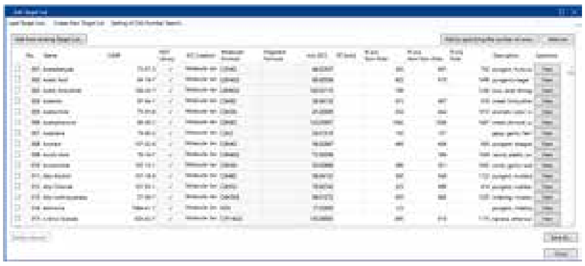
AI structural analysis result window of the flavor component in oyster

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#.

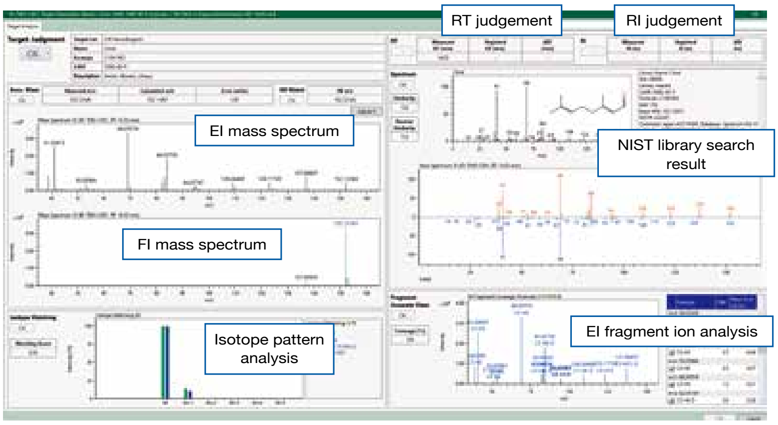
For the data of flavor components in lemon juice, 10 compounds were extracted when searching an off-flavor list that targeted 498 different compounds. The result window on the lower right shows the detailed analysis result of Citral among the 10 components.



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

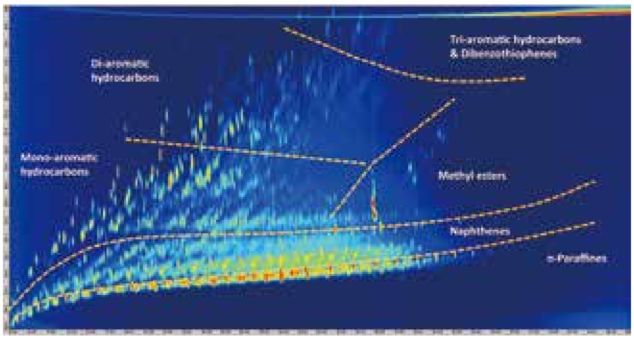


Detailed analysis of Citral present in lemon juice

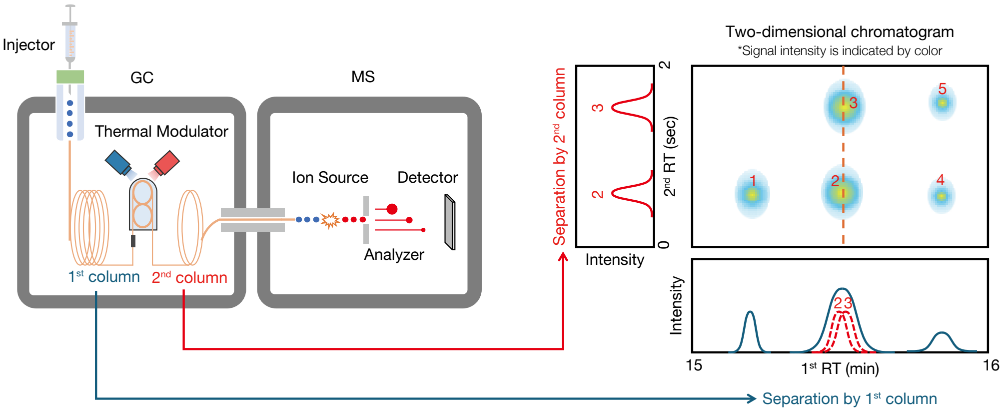
AccuTOF™ GC-Alpha 2.0 with comprehensive 2D GC (GCxGC)

GCxGC is an ultra-high-separation chromatography system that uses two 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 2.0 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 total ion current chromatogram of diesel fuel (EI)

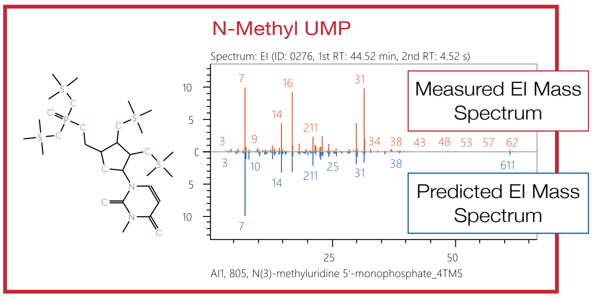


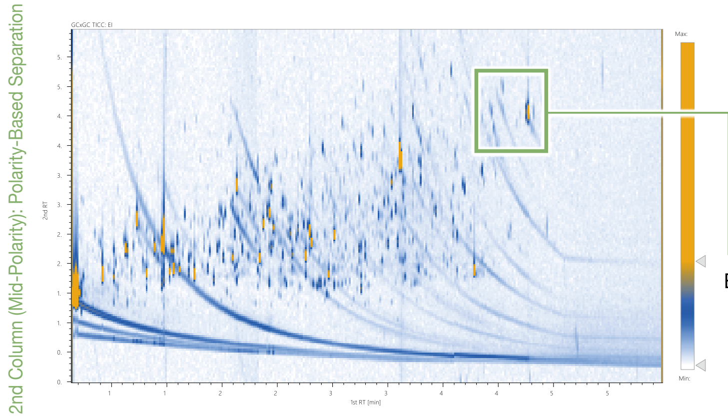
Analysis of Unknown Compounds in HeLa Cells

Water-soluble metabolites in HeLa cells were derivatized with TMS and measured by GCxGC-TOFMS, and a total of 674 metabolites were detected.

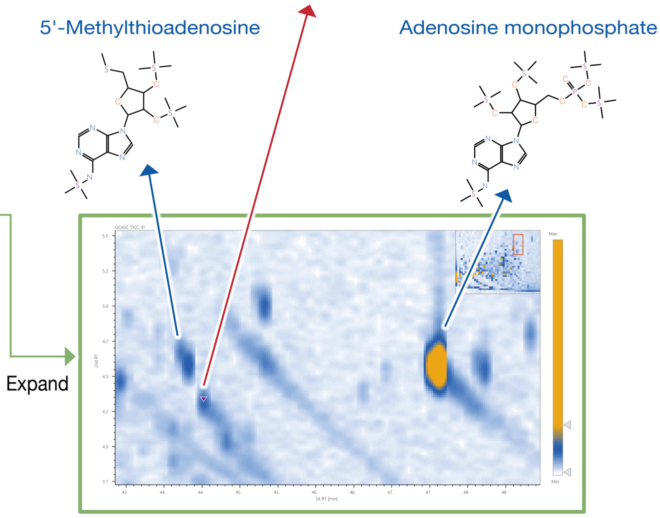
In a previous study2), an unknown compound identified as N-methyluridine monophosphate (N-methyl UMP)—a substance not registered in the NIST database—was subjected to AI-based structural analysis. As a result, N-methyl UMP was obtained as the top candidate, with a good AI score of 805.
In addition, N-methyl UMP and nucleic acid-related compounds have similar retention times in the 2nd column, indicating that they are compounds with similar polarity.

2) Lai Z., Tsugawa H., et al. (2018). Nature Methods, 15(1), 53–56. DOI: 10.1038/nmeth.4512





2D-EI TIC chromatogram



This sample was kindly provided by
Professor Hiroshi Tsugawa of Tokyo University of Agriculture and Technology.

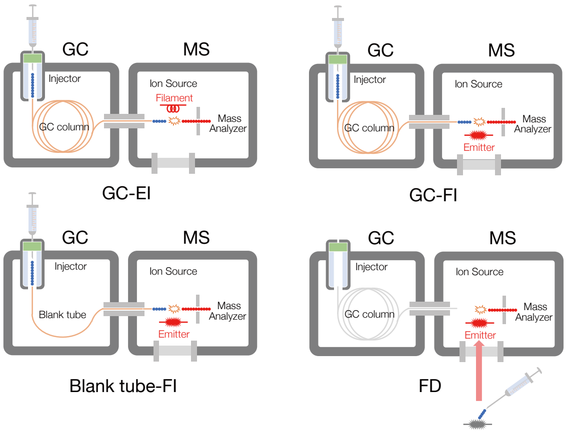
AccuTOF™ GC-Alpha 2.0 for petroleum

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 2.0 is capable of petroleum analysis by three measurement methods.

■ Comparison of the three measurement methods

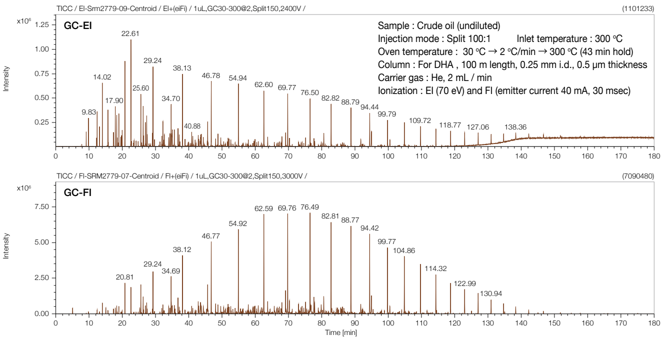
These measurement methods can be used depending on the boiling point range of the sample and the purpose of the analysis. EI/FI/FD combination ion sources can be used for all types of measurements.

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

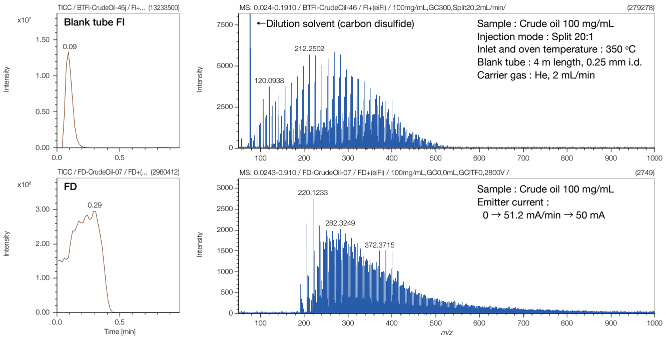
GC/EI and FI methods are suitable for low boiling point components and isomer analysis.The FD method is suitable for type analysis targeting high-boiling components, and the blank tube FI method is suitable for comprehensive analysis of low to high-boiling components.



Sample : Crude oil (undiluted)
Injection mode : Split 100:1 Inlet temperature : 300 °C
Oven temperature : 30 °C → 2 °C/min → 300 °C (43 min hold)
Column : For DHA , 100 m length, 0.25 mm i.d., 0.5 μm thickness
Carrier gas : He, 2 mL / min
Ionization : EI (70 eV) and FI (emitter current 40 mA, 30 msec)

Chromatograms

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



Sample : Crude oil 100 mg/mL
Injection mode : Split 20:1
Inlet and oven temperature : 350 °C
Blank tube : 4 m length, 0.25 mm i.d.
Carrier gas : He, 2 mL/min

Sample : Crude oil 100 mg/mL
Emitter current :
0 → 51.2 mA/min → 50 mA

Chromatograms

Mass spectra

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

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

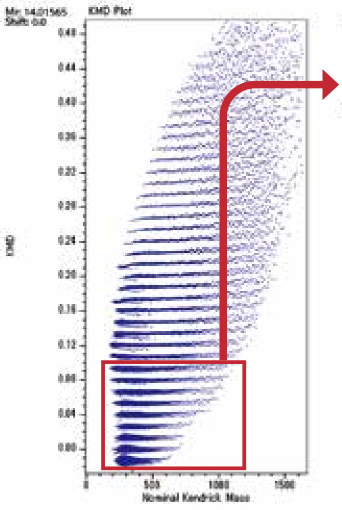
msRepeatFinder can analyze polymers and hydrocarbons, which are composed of repeating units, by visualizing complex mass spectra with KMD plots. The figure on the right shows KMD plots for a FD mass spectrum of crude oil. By visualizing hydrocarbons of different degree of unsaturation, analysis and grouping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

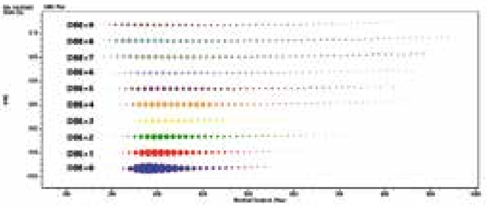
Moreover, by grouping each series, a type analysis calculation can automatically be performed for each group that includes:

- 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_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

AccuTOF™ GC-Alpha 2.0 **with Direct MS**

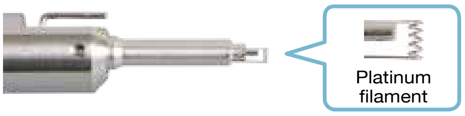
Direct MS mode is useful for the analysis of high-boiling-point and high-mass compounds that are not amenable for GC

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

Compounds that are measured by GC normally have molecular weights below 500 Da, so it is not common to target compounds with molecular weights exceeding 1,000 Da 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 2.0 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)

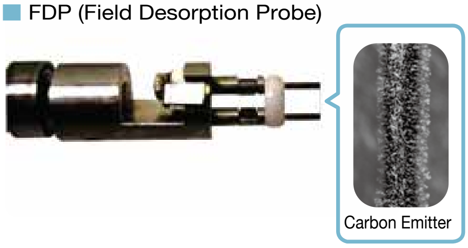


- Sample dissolved or dispersed in solvent is applied to the filament at the tip
- Suitable for high boiling point and/or thermally labile compounds
- Compatible with EI and CI

DIP (Direct Insertion Probe)

- 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)

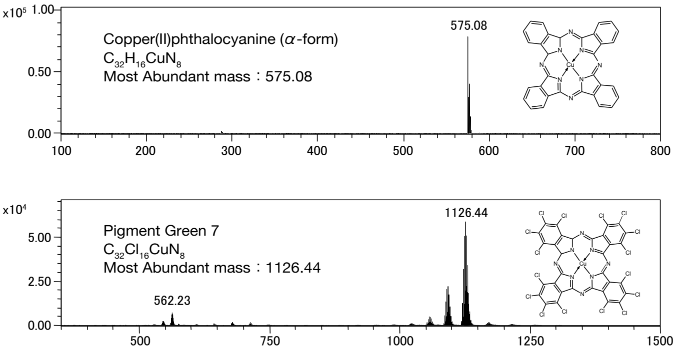


- Sample dissolved or dispersed in solvent is applied to the carbon emitter at the tip
- Suitable for high boiling point, high molecular weight, and/or thermally labile compounds
- Suitable for low- to mid-polar metal complexes
- Used for FD soft ionization

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.

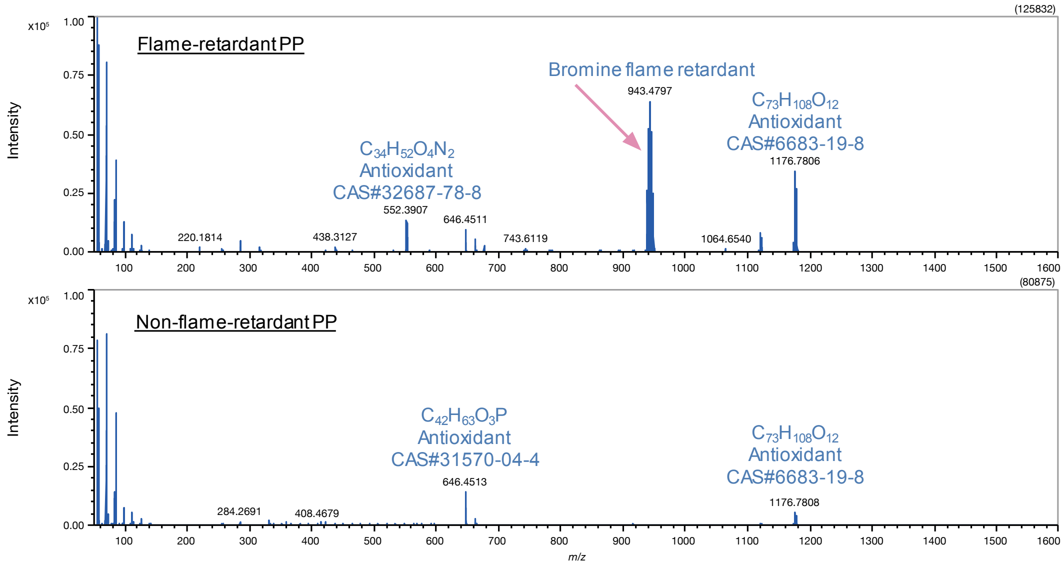
FD Sampling Tool

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

Applying the sample to the emitter

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.

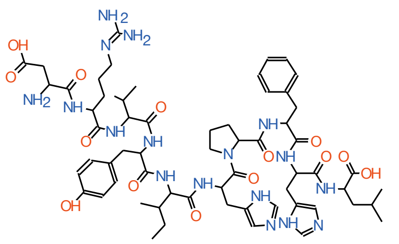
A clear difference peak was detected at *m/z* 943.4797 from the flame-retardant PP. It was estimated to be a brominated flame retardant by isotope pattern analysis and composition estimation.



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

Peptide measurement by FD method (MSTips No.445)

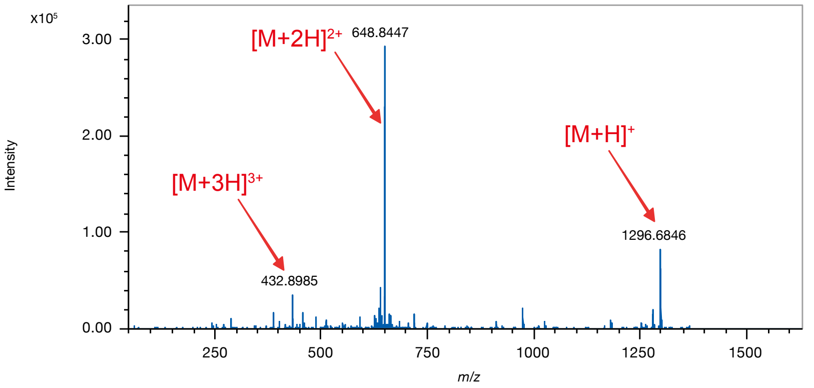
Highly polar compounds that are difficult to measure by GC-MS can also be analyzed by the FD method. Composition formula calculation by accurate mass measurement is also available.



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

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

Structural formula of Angiotensin I

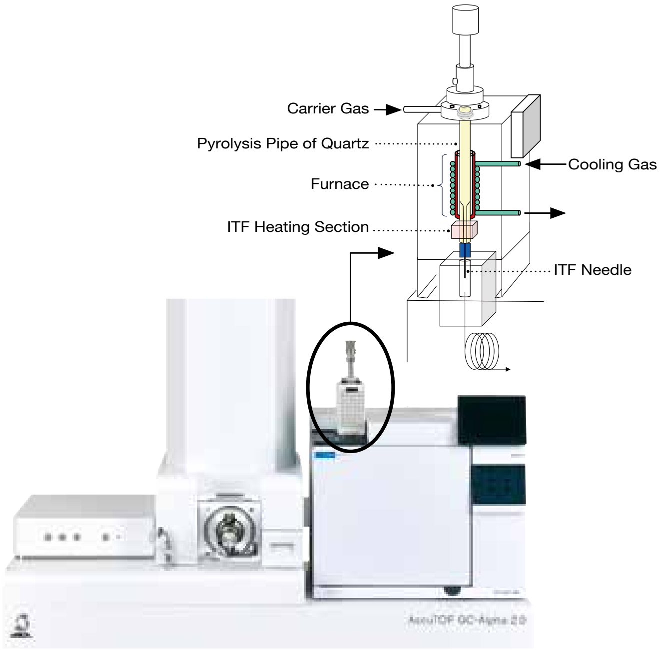


Ion Type	Measured *m/z*	Formula	Calculated *m/z*	Mass Error [mDa]
$[M+H]^+$	1296.68462	C62 H90 N17 O14	1296.68477	-0.15
$[M+2H]^{2+}$	648.84471	C62 H91 N17 O14	648.84602	-1.31
$[M+3H]^{3+}$	432.89845	C62 H92 N17 O14	432.89977	-1.32

FD mass spectrum and accurate mass analysis for Angiotensin I

Sample preparation 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 (EGA/PY-3030D) manufactured by Frontier Laboratories Ltd.

Multi-function Autosampler

■ Multi-function Autosampler

This system can perform various sample introduction methods such as liquid injection, headspace (HS), and solid-phase microextraction (SPME).The photo shows the combination with 2880T by HTA.

Comprehensive 2-Dimensional GC (GCxGC)

■ GCxGC system

This is a continuous heart-cutting system that connects two columns with different polarities in series. Compounds eluted from the first column are trapped by and then periodically released from a modulator, then rapidly analyzed by the second column.

Delivering dramatically higher separation performance than conventional capillary GC, this technique is often referred to as the “ultimate capillary GC method.”

The photo shows an example equipped with the INSIGHT-Thermal Modulator from SepSolve Analytical.

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 STA 2500 manufactured by NETZSCH.

Specification & Configuration

Standard Configuration

Ion Source	Electron Ionization
Analyzer	Dual Stage 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, Windows® Operating System, Main Program (msAxel), Data Analysis Program (msFineAnalysis AI)

Major Options

- EI/FI/FD combination ion source
- EI/PI combination ion source
- CI 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 200 V 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
(0.5 ppm or less hydrocarbon content)

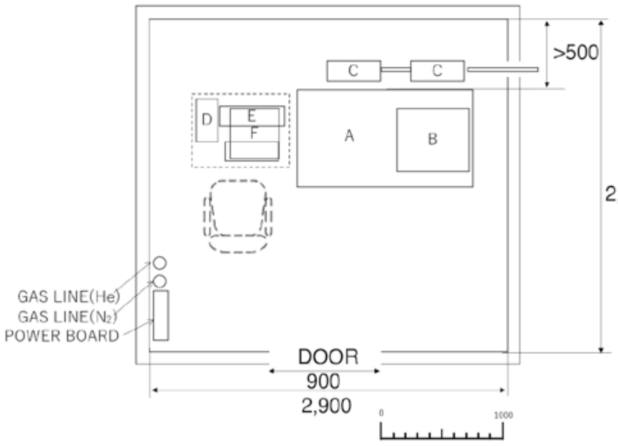
Power supply requirement depends on a specific configuration sold in each territory. Please inquire at a local sales office for details.

Installation Room

Environmental Magnetic Field	Varying magnetic field 1 x 10^{-6} T or less
	Static magnetic field 5 x 10^{-4} T or less
Floor Vibration	Amplitude (p-p) 25 µm 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



Symbol	Unit	W (mm)	D (mm)	H (mm)	Weight (kg)
A	Mass Spectrometer Basic Unit	1,430	790	2.480	348
B	Gas Chromatograph	580	510	490	49
C	Rotary Pumps (per unit)	120	288.5	163	9
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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▼ Local office

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