

Solutions for Innovation

JMS-T200GC

AccuTOF™ GCx-plus

GC-TOFMS & Direct TOFMS
with high speed, high resolving power,
and high mass accuracy.



JEOL Ltd.

High performance and all-round TOFMS

AccuTOF™ GCx-plus

The AccuTOF™ GCx-plus is the most advanced mass spectrometer system of the AccuTOF™ GC series products. The AccuTOF™ GCx-plus provides solutions for a variety of applications.

►► High performance

Reliable determination of elemental composition

The high-resolution and high mass accuracy AccuTOF™ GCx-plus enables accurate elemental composition determination, which is a powerful tool for the qualitative analysis of unknown compounds and impurities.

High-speed data acquisition

The AccuTOF™ GCx-plus performs high throughput analysis using Fast GC with its high-speed data acquisition capability (50 spectra/s). It also supports GCxGC for ultrahigh separation analysis.

►► All-round

A variety of ionization and sample introduction techniques

While electron ionization (EI) is effective in acquiring structural information, detection of molecular ions is critical in qualitative analysis of unknown compounds.

In addition to chemical ionization (CI), the AccuTOF™ GCx-plus supports field ionization (FI), field desorption (FD), and photoionization (PI), which are powerful soft ionization techniques for molecular ion detection.

The system also supports direct sample inlets for analysis of high boiling point compounds and rapid analysis.

The AccuTOF™ GCx-plus is a superior gas chromatograph time-of-flight mass spectrometer (GCTOFMS) system that simultaneously accomplishes high-resolution analysis, high mass accuracy, and high-speed data acquisition.

AccuTOF™ GCx-plus

AccuTOF™ GCx

AccuTOF™ GCv 4G

AccuTOF™ GCv

AccuTOF™ GC

Solutions provided by AccuTOF™ GCx-plus

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A wide range of applications

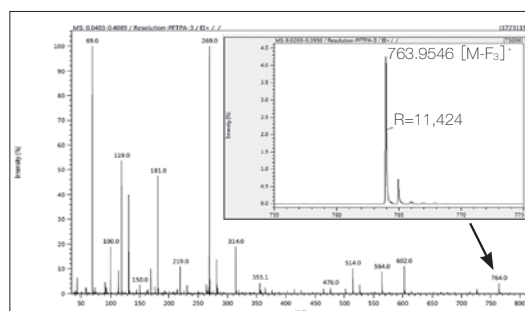
Elemental composition determination by accurate mass analysis



Accurate results for reliable elemental composition determination

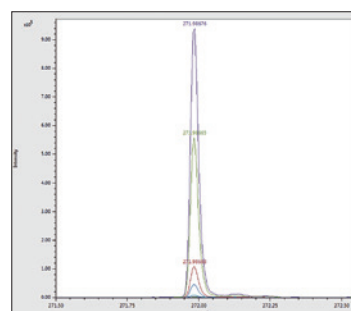
The AccuTOF™ GCx-plus consistently acquires high resolution, high mass accuracy, and high sensitivity data for long periods of time. It also achieves high mass accuracy from low intensity peaks, facilitating reliable determination of elemental compositions. Furthermore, the AccuTOF™ GCx-plus, with its wide dynamic range, can easily analyze compound mixtures at different concentrations.

High resolution



El mass spectrum of perfluorotriptylamine

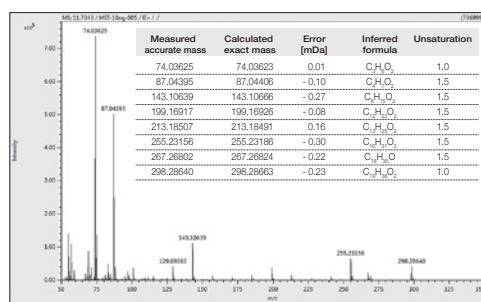
High mass accuracy 1 (at different concentrations, single ion)



	Amount of injection [pg]	Error [mDa]
1:	0.1	0.26
2:	0.5	0.54
3:	1	0.34
4:	5	-0.56
5:	10	-0.04
6:	50	0.07
7:	100	0.21
8:	500	-0.02
9:	1000	0.08

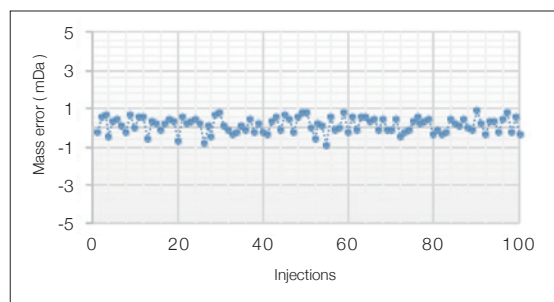
El mass spectrum of octafluoronaphthalene (zoomed around m/z 272) and m/z measurement errors of the molecular ion at various injection amounts

High mass accuracy 2 (single component, multiple ions)



El mass spectrum of methyl stearate and accurate mass measurement results of the major ions

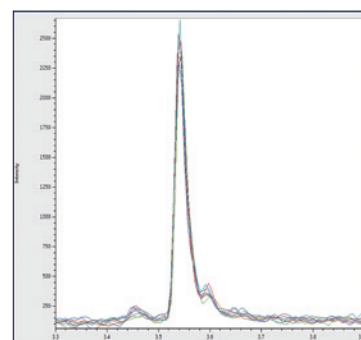
Stable mass accuracy over time



m/z measurement errors of the molecular ion of octafluoronaphthalene (OFN; m/z 271.9867) when 100 fg of OFN was repeatedly measured for 100 times (GC column bleeding at m/z 281.0511 was used as the internal mass reference)

High sensitivity / Wide dynamic range

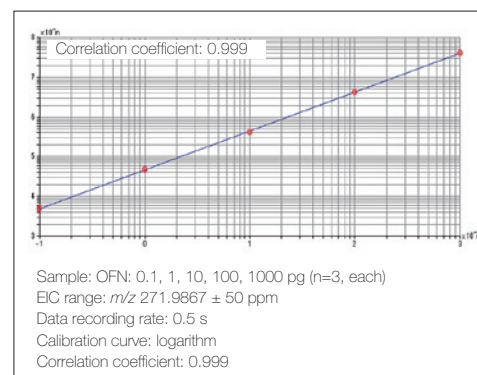
100fg CV=5.2%, IDL=16fg



Injection no.	Peak area
1	65745
2	67212
3	58394
4	70698
5	65897
6	65604
7	65994
8	65230
CV(%)	5.2
IDL(fg)	16

100 fg of octafluoronaphthalene (OFN) was measured continuously 8 times. From the standard deviation of the EIC peak areas of OFN molecular ions, an instrument detection limit (IDL) of 16 fg was calculated. CV: Coefficient of variation IDL: Instrument detection limit

Linear response > 1x10⁴

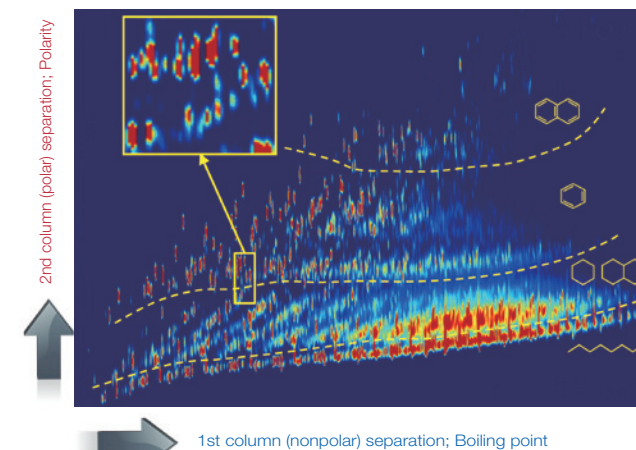


A 4 order linear response was verified by measuring 100 fg to 1,000 pg of OFN. The wide dynamic range is critical for accurate qualitative/quantitative analysis.

GCxGC analysis by ultrahigh speed data acquisition

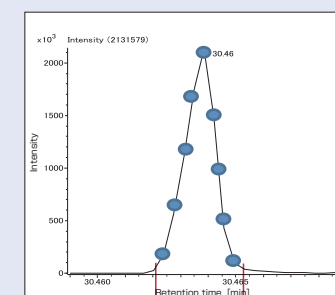
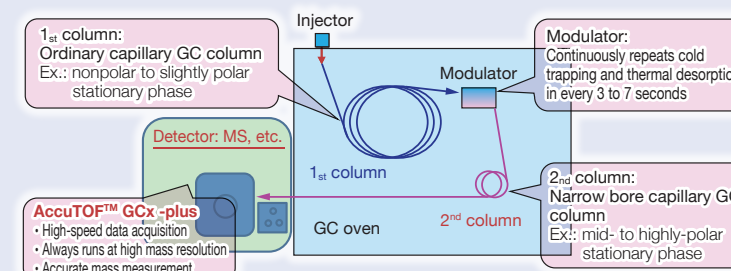
Accurate mass measurements are easily accomplished in GCxGC analysis, which requires ultrahigh speed data acquisition. This is especially effective for nontargeted qualitative analysis of trace components.

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



Ultrahigh separation analysis GCxGC (comprehensive 2D GC)

GCxGC is an ultrahigh separation chromatography system designed to use 2 columns having different polarities, trap the eluted components using a modulator at the end of the 1st column at given intervals, and perform high-speed analysis of the trapped components in 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 analysis of components by group. 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.



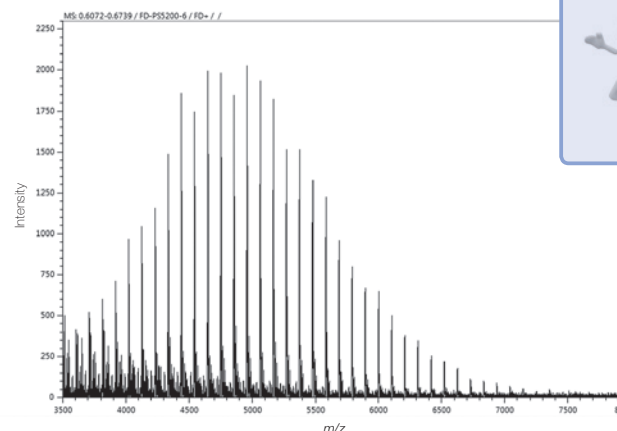
Peak width: 0.18 s

9 data points

At a data acquisition speed of 50 spectra/s, the AccuTOF™ GCx-plus is capable of ultrahigh separation GCxGC analysis while maintaining ample data points across each chromatographic peak.

Wide mass range

FD mass spectrum of polystyrene 5200



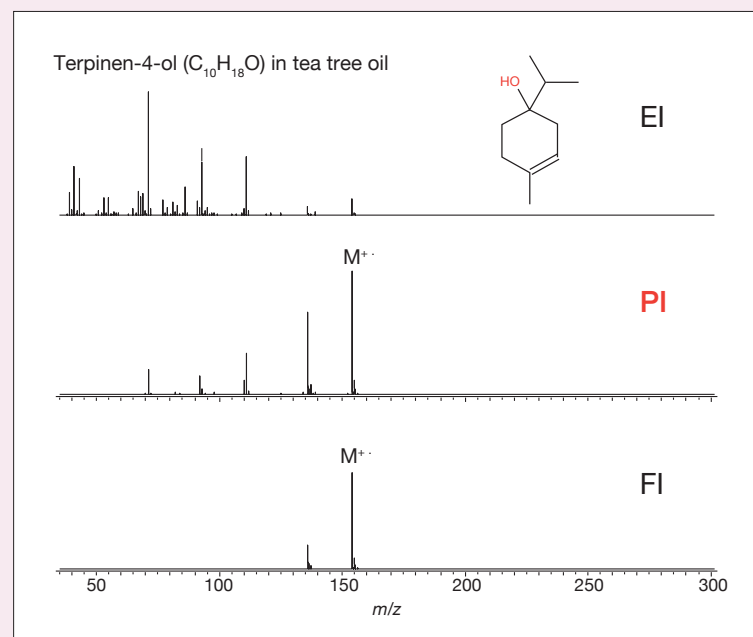
Oligomer analysis with direct MS

The AccuTOF™ GCx-plus, with a wide mass range and direct inlet system, can analyze samples with large molecular weights that are difficult to handle with GC.



Why are multiple ionization techniques critical in GC/MS?

EI, the most widely used ionization technique in GC/MS, is superior in sensitivity and reproducibility. It is also supported by an immense database.



For any scientist using GC/MS in search of further information, what is ultimately important is molecular ion detection. EI, using 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. On the AccuTOF™ GCx-plus, FI, PI, and CI are optionally available as soft ionization techniques. 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 ionization techniques with a low level of internal energy in molecular ions compared to EI and CI. Being soft ionization techniques with minimum fragmentation, FI and FD are ideal for molecular weight determination.

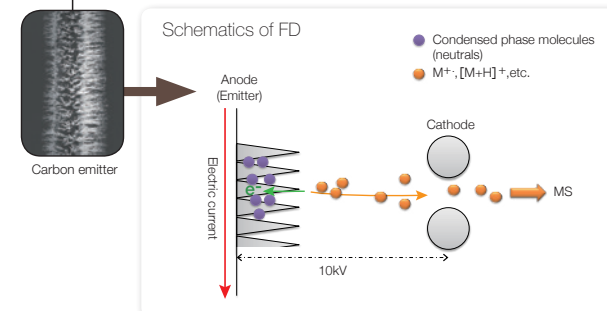
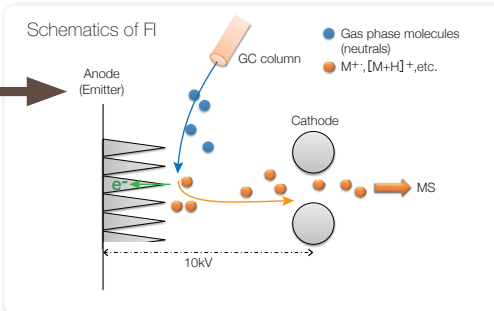
FI (Field Ionization)

- ▶ 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)

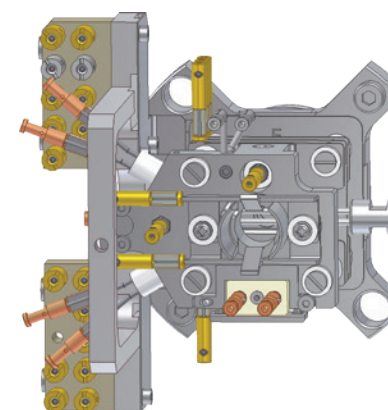
- ▶ The sample is applied onto the emitter and directly introduced to the system.
- ▶ Suitable for analysis of thermally labile compounds.
- ▶ Ideal for samples soluble in nonpolar solvents.
- ▶ Analyzes powder samples dispersible in solvents.
- ▶ Analyzes low- to mid-polar metal complexes.
- ▶ Analyzes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

Tip of the FD probe



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

EI / FI / FD combination ion source (optional)



Features

A single ion source supports EI (hard ionization) and FI/FD (soft ionization) techniques. Switching between EI and FI/FD is simple and quick.

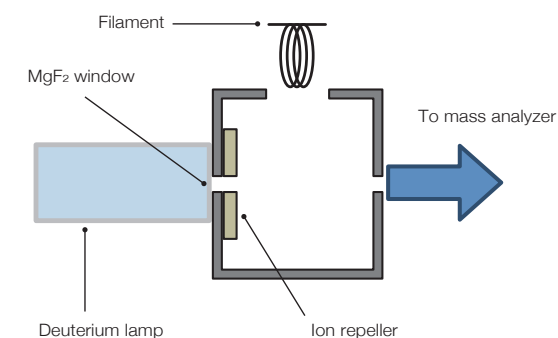
- ▶ No need to change the ion source
- ▶ No need to change the GC-interface
- ▶ No need to break vacuum

Effective use of EI/FI/FD:

- ▶ EI for qualitative analysis through library search
- ▶ FI for molecular weight determination
- ▶ GC/FI for type analysis of hydrocarbon samples
- ▶ FD for polymer analysis
- ▶ Accurate mass measurement

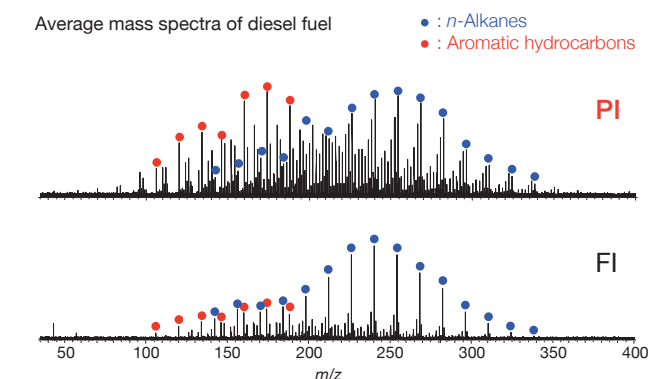
PI (Photoionization) ~ EI / PI combination ion source

The PI Ion Source adds a vacuum ultraviolet light source to the standard EI Ion source, enabling photoionization.



Schematics of the ion source

Aromatic hydrocarbons, which strongly absorb UV light, are preferentially ionized with PI, making the technique useful for detecting aromatic hydrocarbons in a complex mixture.



CI

Optional CI source comes with 3 different reagent gas lines, eliminating a lengthy process of reagent gas selection.

Direct sample inlet system (optional)

2 types of direct sample inlet probes for different applications

- ▶ EI and CI supported



DEP (Direct Exposure Probe)

Ideal for high boiling point/thermally unstable compounds. The sample, which is dissolved in a solvent, is applied to the filament at the tip.



DIP (Direct Insertion Probe)

Ideal for high boiling point compounds/samples insoluble in solvent. A solid sample can be directly introduced to a dedicated glass sample tube for analysis.

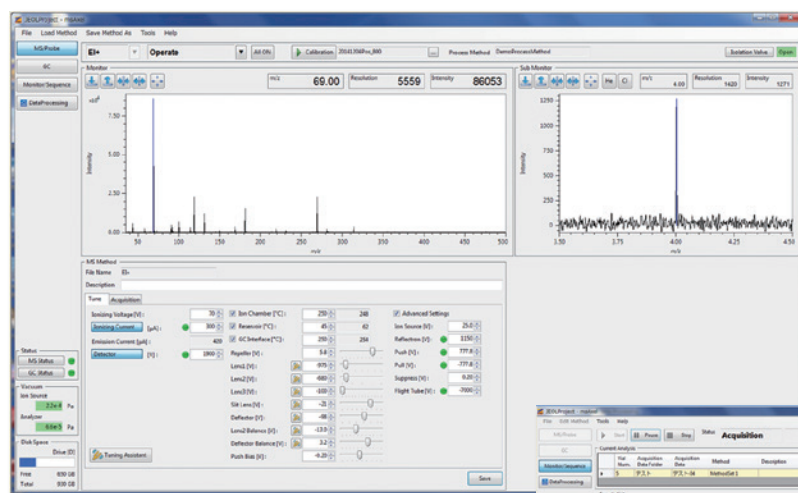


Load-lock flange for DIP/DEP/FDP

AccuTOF™ GCx-plus main program “msAxel”

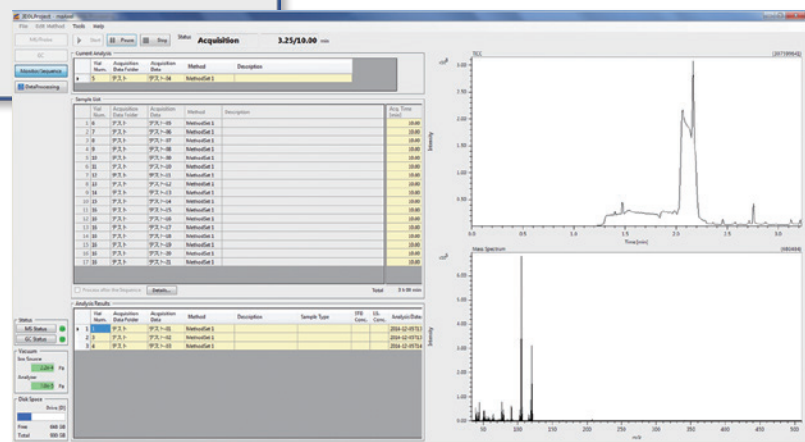
1 Auto tuning by Tuning Assistant

- Accomplishes high performance tuning without a lengthy manual process.
- Facilitates easy acquisition of optimum sensitivity/resolution in all ionization modes (EI, CI, FI, FD, PI).



2 Powerful automated functions

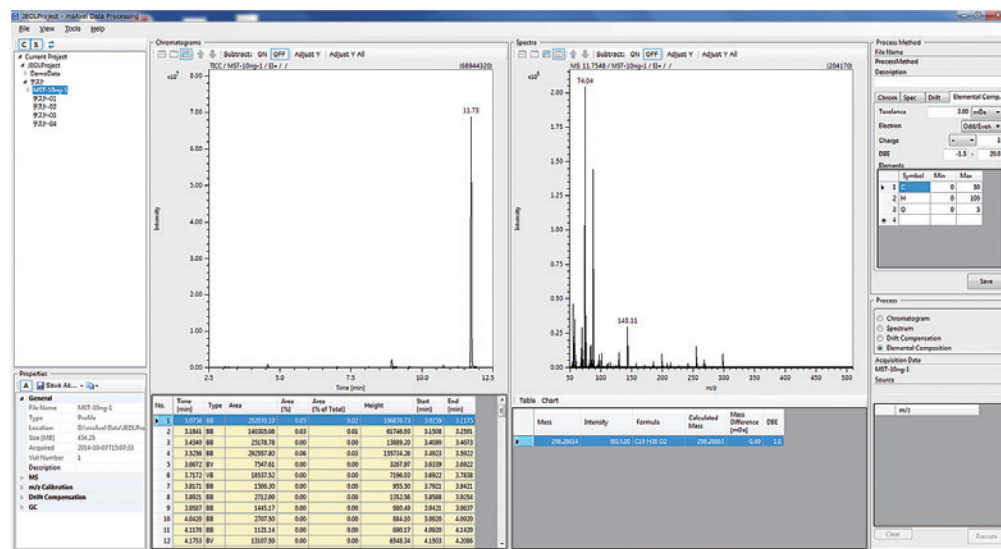
- Auto drift correction
Automatically performs drift correction on every spectrum in acquired data.
- Auto data conversion
Automatically converts acquired data to netCDF format.
- Auto data transfer
Automatically transfers acquired data to any location (PC for data analysis, etc.)



3 Interactive views

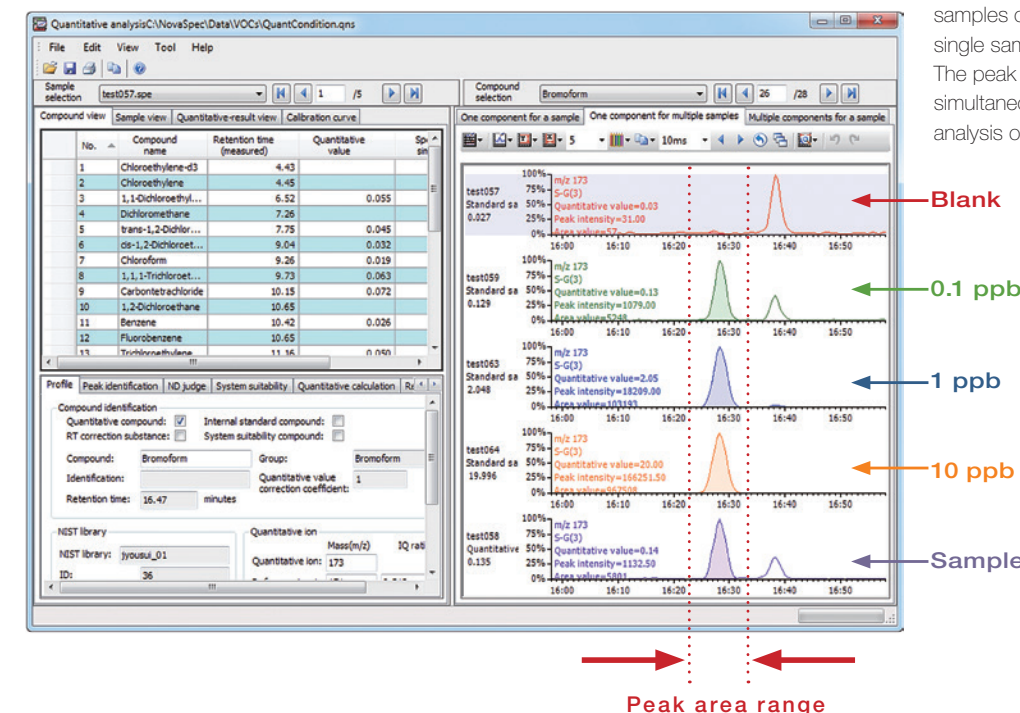
Chromatograms and mass spectra on a single view. Elemental composition determination using exact mass on the same view.

Other features, including isotopic peak pattern simulation, elemental composition determination, and calibration table editor, can be arranged as the user wishes.



Software for simultaneous quantitative analysis of multiple components - “Escrime”

Escrime is designed to calculate EIC peak areas, plot calibration curves, and determine quantitative values. With further manipulation of the resulting data including separate or collective editing of area calculation ranges, this software significantly speeds up the quantitation process.



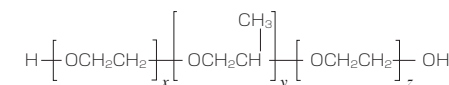
Peaks of the components contained in multiple samples or peaks of multiple components in a single sample can be presented on a single view. The peak area calculation ranges can be simultaneously changed, allowing for batch analysis of more than 150 samples.

Polymer analysis software “Polymerix”

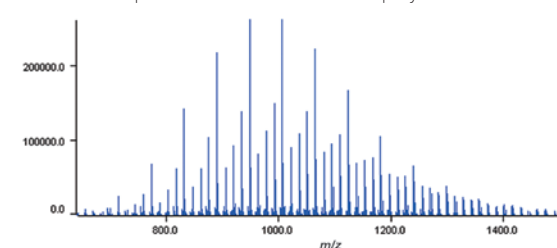
FD mostly forms ions that reflect the molecular weights of analytes through the formation of M^+ , $[M+H]^+$ and $[M+Na]^+$, thus allowing for the calculation of the average molecular weight, degree of polymerization, and polydispersity from the m/z and the intensity of each peak. Polymerix is designed to calculate the average molecular weight, degree of polymerization, and polydispersity of polymers, and estimate the repeated structure and end groups from the data acquired in FD and FI.

The example below is a visualization of the relative abundance (distribution) of each molecule in an ethylene oxide/propylene oxide (EO/PO) block copolymer. Polymerix easily calculates the average molecular weight and polydispersity.

EO/PO block copolymer



FD mass spectrum of EO/PO block copolymer



Molecular distribution of EO/PO block copolymer

Repeat B, EO: (C ₂ H ₄ O) _n											
	0	1	2	3	4	5	6	7	8	9	10
6											
7											
8											
9											
10											
11	2.65	3.42									
12	9.58	10.37	1.63	2.17	1.08	1.66	1.27	1.33	1.61		
13	25.98	23.80	23.46	24.20	23.93	17.79	12.39	7.36	6.81	3.56	2.24
14	54.36	39.41	35.20	31.16	26.41	20.61	13.98	9.37	7.03	4.81	2.82
15	83.18	62.75	43.08	34.49	28.19	19.84	14.31	9.97	6.35	2.97	2.14
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 : Number average molecular weight
Mw : Weight average molecular weight
Mz : Z average molecular weight
PD : Polydispersity index (Mw/Mn)

AccuTOF™ GCx-plus

► Automatic isolation valve

Allows for changing/cleaning of the ion source while maintaining high vacuum in the mass analyzer

► High response detector

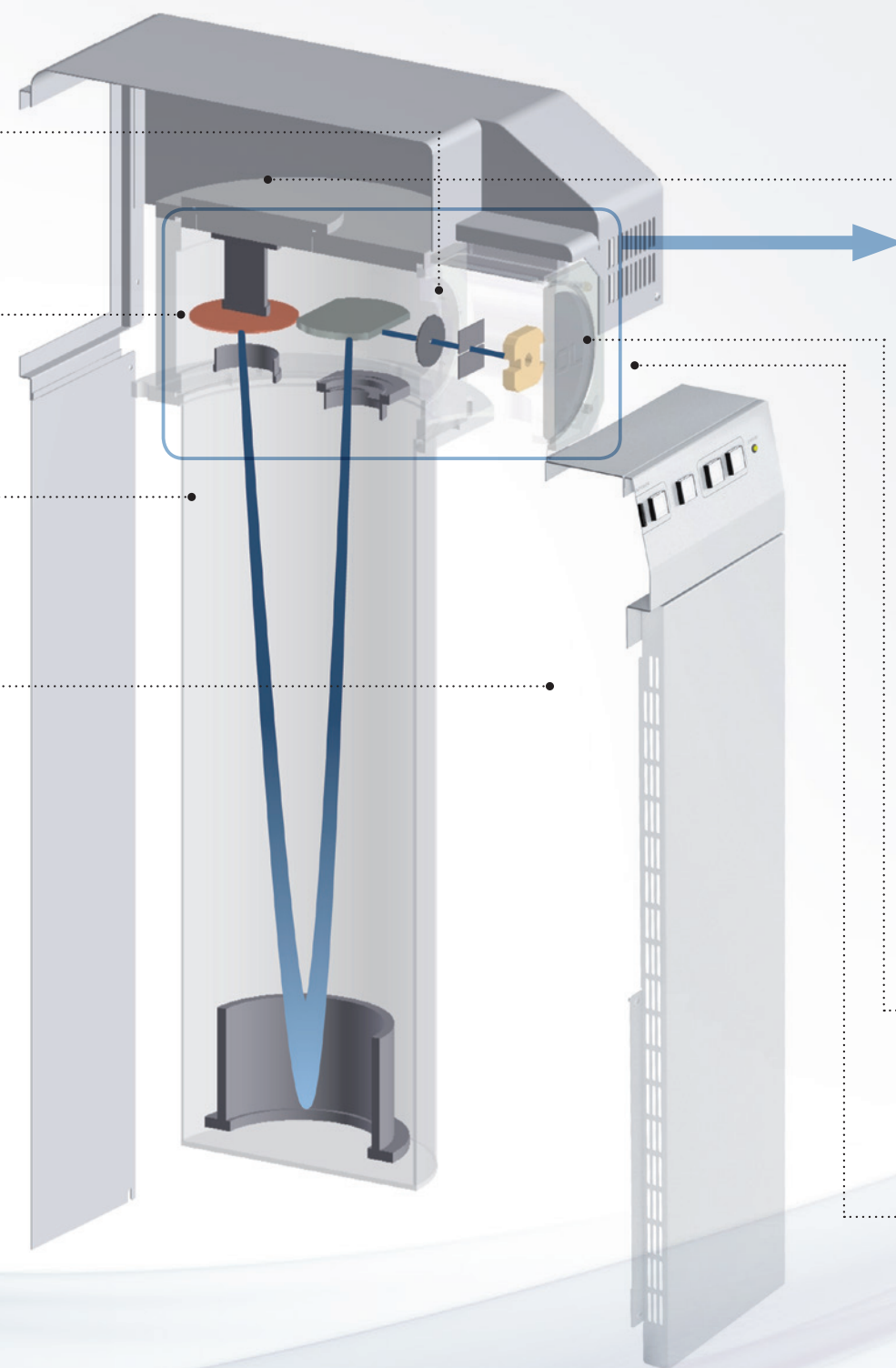
High speed MCP detector unit with enhanced response

► Mass analyzer

Flight tube with enhanced thermal stability; maintains high mass accuracy

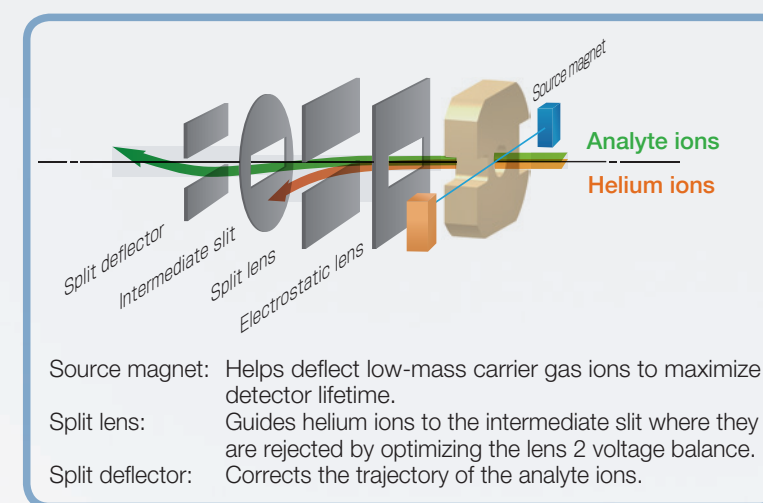
► High vacuum system

Fully integrated in the spectrometer console
2 turbo molecular pumps
2 rotary pumps



Standard EI ion source and ion transfer system

Successfully eliminates 99.9% or more of He ions.
Stable high-transmission-rate (=high sensitivity) ion transfer system maximizes detector lifetime.
(Patent JP3967694, US7034288, GB2404080)



► Gas Chromatograph

(Agilent 7890B)

► Digitizer

Insures a 4 order dynamic range by the 4 GHz digitizer (ADC) and high performance data acquisition system

► Direct inlet flange

Supports analysis by GC and direct sample introduction (DIP, DEP, FDP) techniques

New!

► Auto-reservoir

Mass reference compounds and volatile samples can be introduced automatically for easier accurate mass measurements.



How does the AccuTOF™ GCx-plus support a wide range of applications?

The AccuTOF™ GCx-plus can be equipped with various direct sample inlet systems in addition to the standard GC/MS interface, allowing analysis of both volatile and high-boiling point analytes. FI, FD, and PI, which are unique to AccuTOF™ GCx-plus, further expand applications. AccuTOF™ GCx-plus will provide solutions to your challenging problems.



Application 1 Chemistry p12

1. Analysis of organic electro-luminescence material
2. Analysis of fullerenes

Application 2 Material Science p13

1. Analysis of a photopolymerization initiator
2. Analysis of antioxidant
3. Analysis of pigments
4. Analysis of ionic liquid
5. Analysis of fluorinated compound



Application 8 Petroleum Products p20

1. Ultrahigh separation analysis of diesel fuel with GCxGC
2. Type analysis of microcrystalline wax with FD

Application 3 Polymers p15

1. Pyrolysis GC/MS of acrylic resin
2. Thermal extraction GC/MS of additives in a resin
3. FD analysis of polystyrene



A wide range of applications

Application 7 Fragrances p19

1. GCxGC/TOFMS analysis of tea tree oil
2. GCxGC/TOFMS analysis of rose oil



Application 4 Environmental Science p16

1. Analysis of PCBs in oil



Application 6 Metabolites p18

1. Analysis of fatty acid methyl esters (FAMES)
2. Analysis of isomeric disaccharides



Application 5 Food Safety p17

1. Analysis of agrochemical residues in food



Chemistry



Rapid analysis within a minute with direct sample inlets

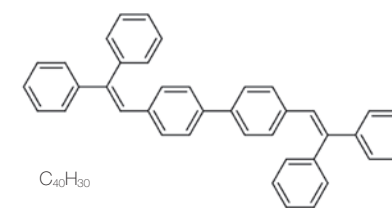
Direct sample introduction with FDP, DIP, or DEP, is optimum for confirming synthesized organic compounds since the measurement is quick and accurate mass can be obtained. Direct sample inlets are also suitable for high boiling point analytes.

1. Analysis of organic electro-luminescence material

An organic electro-luminescence compound was analyzed with a combination of DEP and EI (a.k.a., Desorption EI, or DEI) and with FD.

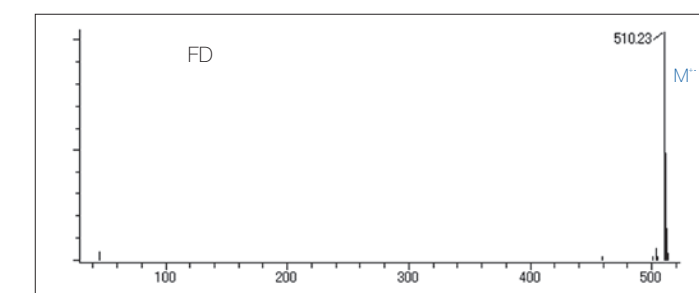
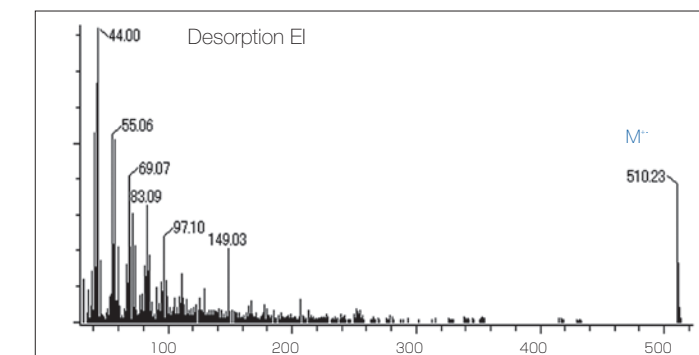
Analysis time was within 1 minute for either method. Elemental composition was confirmed with measured accurate mass with either method.

The FD mass spectrum was simpler and suitable for molecular weight confirmation.



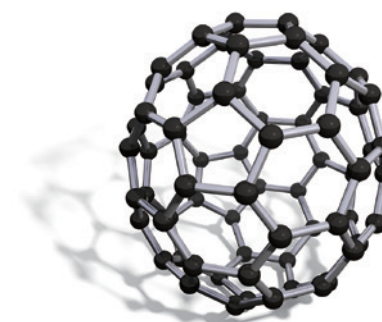
Measured accurate mass	Calculated exact mass	Error [mDa]	Inferred formula
510.23380	510.23420	-0.40	C ₄₀ H ₃₀

Mass spectra of organic electro-luminescence compound

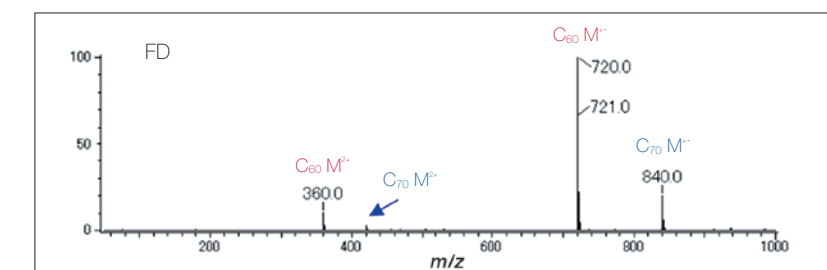
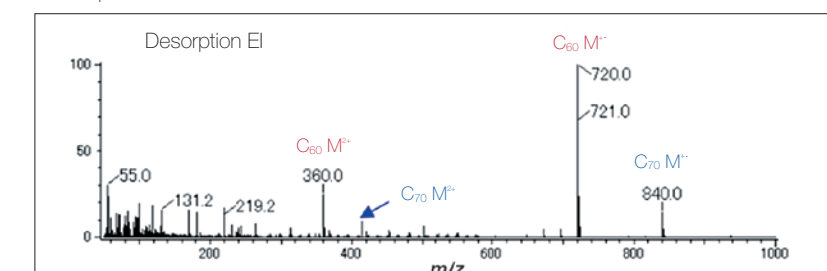


2. Analysis of fullerenes

A mixture of fullerenes was analyzed with DEI and FD. With DEI, the mass spectrum was more complex with fragment ions. With FD, it was easy to conclude that the sample was a mixture of C₆₀ and C₇₀.



Mass spectra of fullerenes





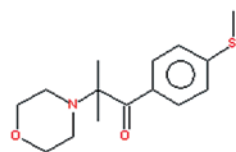
Application 2

Material Science

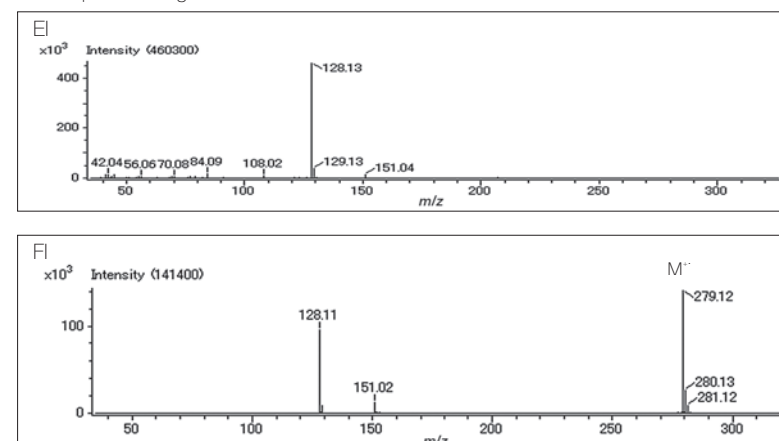
1. Analysis of a photopolymerization initiator

Irgacure 907, a α -aminoalkylphenolic photopolymerization initiator, does not show molecular ion at all with EI. With FI, the molecular ion is easily observed.

Irgacure 907
C₁₅H₂₁NO₂S Mw : 279.12930



Mass spectra of Irgacure 907



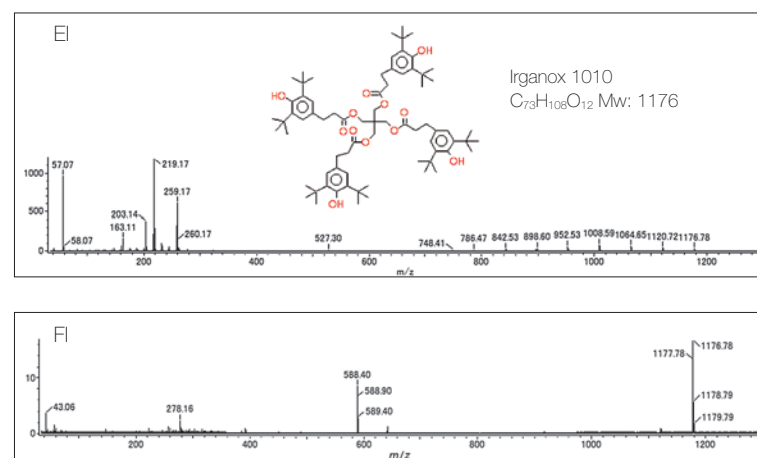
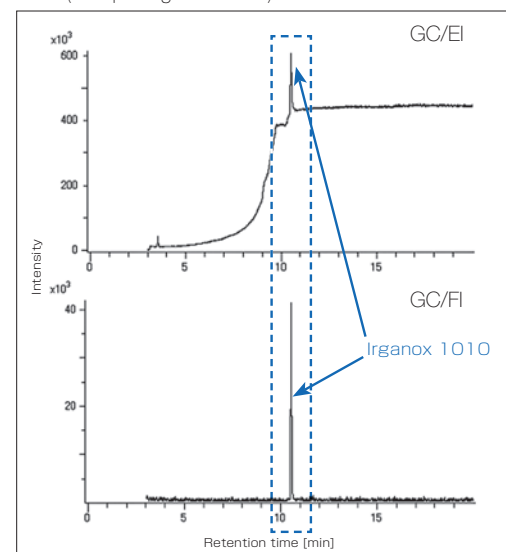
Why is EI alone not sufficient?

EI mass spectra can be searched against mass spectral libraries and elemental compositions of the observed ion can be inferred. However, a compound cannot be identified if the molecular ion is not detected and there is no meaningful hit in the library search. It is absolutely important to detect molecular ions with soft ionization methods such as FI and PI. Identification of unknowns is made quick and reliable with the EI/FI/FD combination ion source or EI/PI combination ion source.

2. Analysis of a high-boiling-point compound (antioxidant) (MS Tips No. 123)

Since FI does not ionize column bleed, the TICC clearly shows the high-boiling-point compounds.

TICC (Sample: Irganox 1010)



High quality GC/MS interface with no cold spot

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

Irganox and Irgacure are trademarks of BASF.

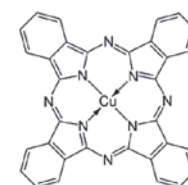


Analysis of samples of various states

Pigments and an ionic liquid, which are insoluble or non-volatile and not amenable for GC, were analyzed in minutes and their molecular weights determined.

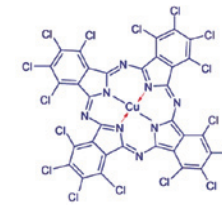
3. Analysis of pigments

Using FD ionization, the AccuTOF™ GCx-plus detected molecular ions for the refractory and insoluble pigments.



C₃₂H₁₆CuN₈
Mw : 575.07939

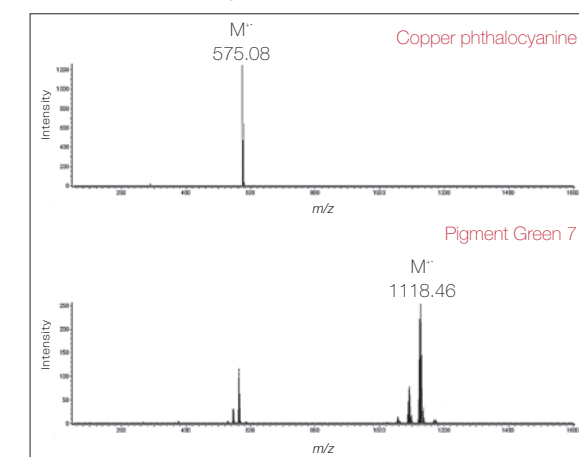
Copper phthalocyanine (top)



C₃₂Cl₁₆CuN₈
Mw : 1118.45584

Pigment Green 7 (bottom)

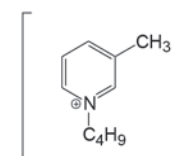
FD mass spectra of pigments



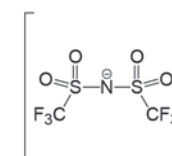
4. Analysis of an ionic liquid sample (MS Tips No. 113)

FD makes it easier to detect cations and cluster ions. Further accurate-mass analysis allows for determination of the elemental formula of each compound.

Cationic compound (C) :
Pyridinium compound

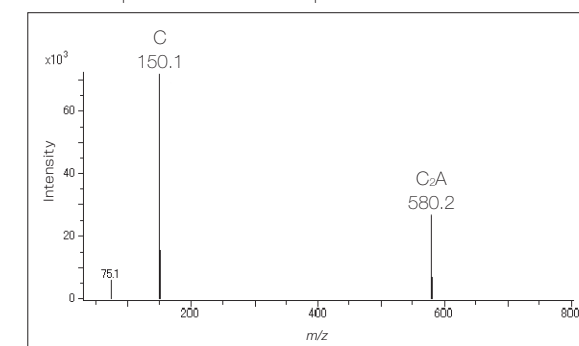


Anionic compound (A) :
Fluorinated compound (triflate)



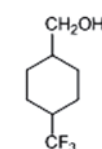
Ionic species	Measured accurate mass	Calculated exact mass	Error [mDa]	Inferred formula
C	150.12887	150.12827	0.60	C ₁₀ H ₁₆ N
C ₂ A	580.17664	580.17384	2.80	C ₂₂ H ₃₂ F ₆ N ₃ O ₄ S ₂

FD mass spectrum of an ionic liquid



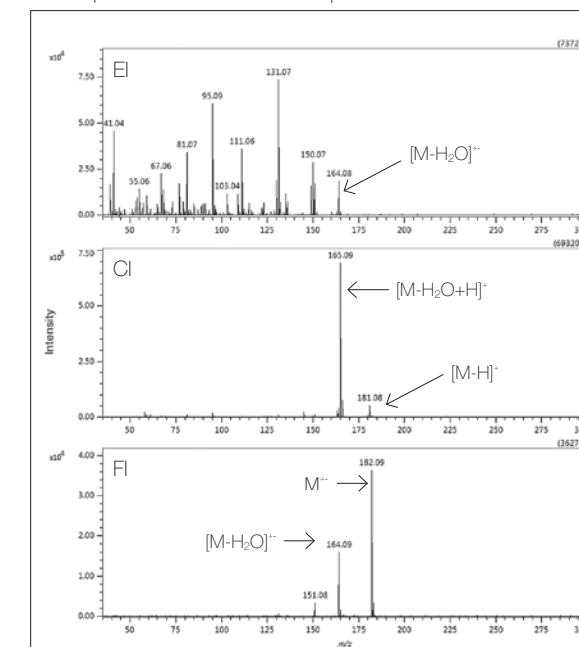
5. Analysis of fluorinated compound

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
C₈H₁₃F₃O
Mw : 182.09185

Mass spectra of a fluorinated compound



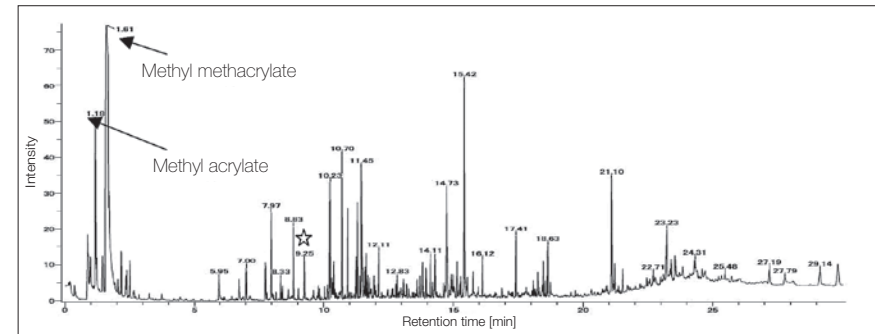


Application 3
Polymers

1. Pyrolysis GC/MS of acrylic resin (MS Tips No. 101)

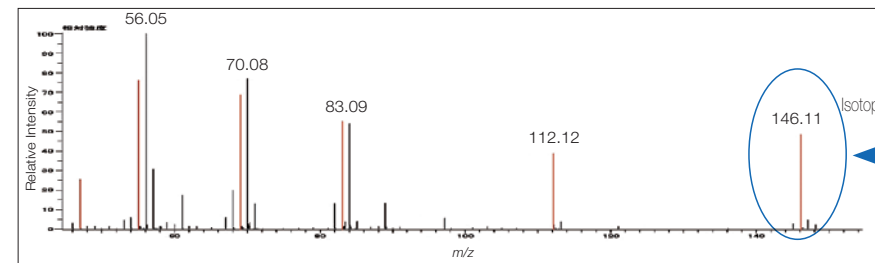
Pyrolysis GC/MS is widely used as an analytical technique for high molecular weight polymers. Instant thermal decomposition makes it a simple yet powerful technique with high reproducibility.

TICC of acrylic resin Pyrolysis GC/EI/TOFMS

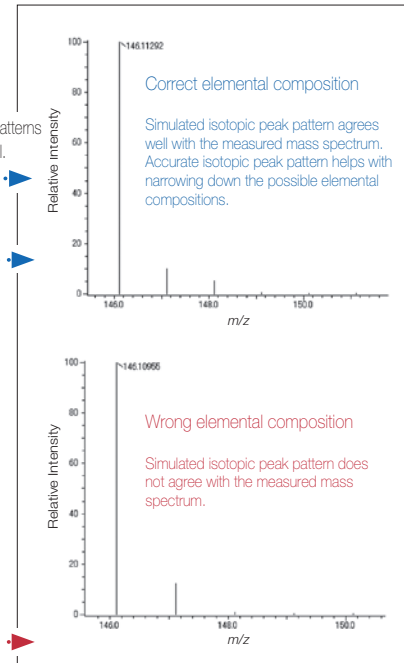


GC/TOFMS, which is capable of acquiring exact-mass results in a single GC/MS analysis, enhances the reliability of library search results. It is also effective for qualitative analysis of peaks that cannot be identified through a library search. The system also acquires an accurate distribution of isotopes for molecular ions, which is effective in molecular identification.

EI mass spectrum of Peak at 9.25 min (☆ on the TICC above)



Simulation of isotope pattern



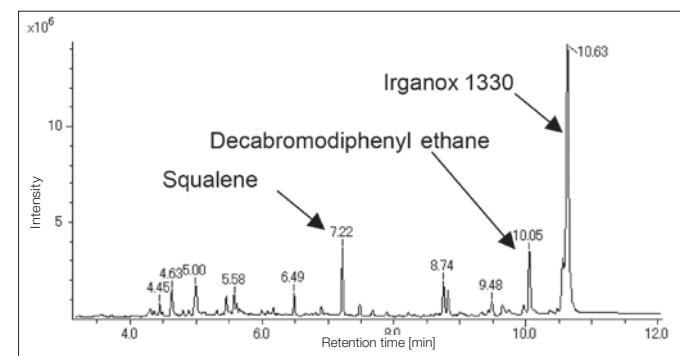
Elemental composition determination

Measured accurate mass	Calculated exact mass	Error [mDa]	Inferred formula	Unsaturation
46.99437	46.99555	-1.18	CH ₃ S	1.5
55.05387	55.05478	-0.90	C ₄ H ₇	1.5
69.06963	69.07043	-0.80	C ₆ H ₉	1.5
83.08569	83.08608	-0.39	C ₆ H ₁₁	1.5
112.12456	112.12520	-0.64	C ₈ H ₁₆	1.0
146.11280	146.11292	-0.12	C ₈ H ₁₈ S	1.0
	146.10955	3.25	C ₁₁ H ₁₄	5.0

2. Thermal extraction GC/MS of additives in a resin (MS Tips No. 138)

Using thermal extraction GC/TOFMS, the system analyzed additives in a resin. Additives detected were squalene, decabromodiphenyl ethane (bromine flame retardant), Irganox 1330 (antioxidant).

TICC of the thermal extraction GC/MS of a resin



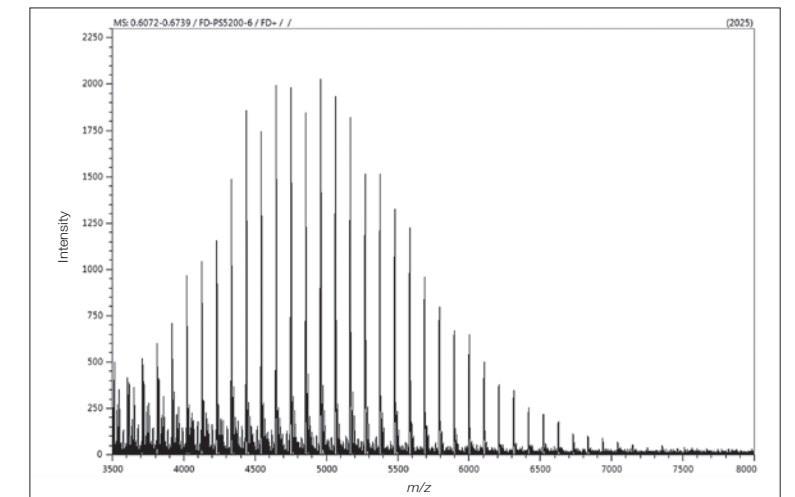
3. Calculating the average molecular weight of polystyrene using FD

The mass spectrum acquired from polystyrene 5200 using FD ionization shows ions at m/z 6500 or higher. The AccuTOF™ GCx-plus is effective for polymer analysis in the oligomer range in addition to GC/MS analysis. For FD ionization, the system is capable of speedy data acquisition within 1 minute.

Mn	Mw	PD	DPn	DPw
4928.9	5309.4	1.1	46.8	50.5

Mn : Number average molecular weight
Mw : Weight average molecular weight
PD : Polydispersity
DPn : Number average degree of polymerization
DPw : Weight average degree of polymerization

FD mass spectrum of polystyrene 5200



Why is the AccuTOF™ GCx-plus highly useful for polymer analysis?

Pyrolysis/GC/MS is a widely used technique for polymer analysis. However, many of the pyrolysis products of even a common polymer are not in an EI mass spectral library. The AccuTOF™ GCx-plus helps with identifying pyrolysis products by determining molecular weights with various soft ionization techniques and elucidating elemental compositions with accurate mass measurements. With FD, an oligomer, which is not amenable to GC/MS, can be directly analyzed. Its average molar masses and polydispersity index can be obtained by processing the FD mass spectrum with polymer analysis software.



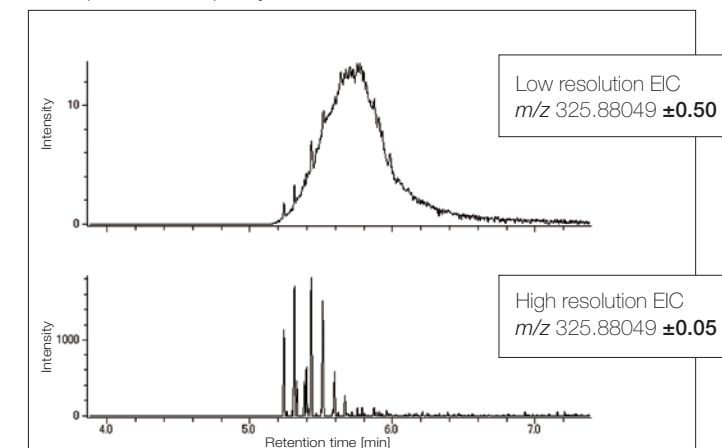
Application 4

Environmental Science

Analysis of PCBs in oil (FastGC) (MS Tips No. 130)

High selectivity at high resolution makes it possible to detect the PCBs contained in an oil sample.

EIC of pentachloro biphenyls in a transformer oil



The EICC acquired with the window width set to low resolution (top, equal to QMS) was unable to eliminate the oil interference from the PCB impurities. The high-resolution mass chromatogram (bottom) successfully detected the peaks of pentachlorinated PCBs by eliminating the interference.



Application 5

Food Safety

Analysis of agrochemical residues in food

High selectivity

High-resolution TOFMS can reduce the interference from matrix. Peaks from the matrix that are detected at low resolution will be eliminated at high resolution. This high selectivity reduces false positives and allows for more accurate quantitation.

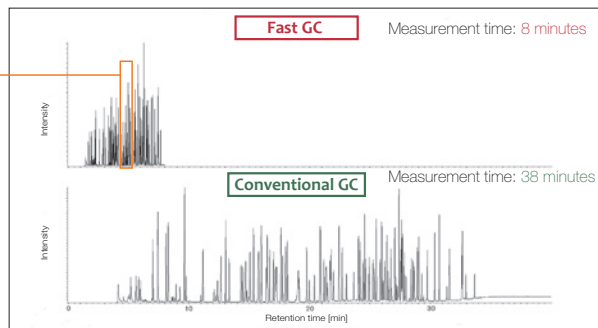
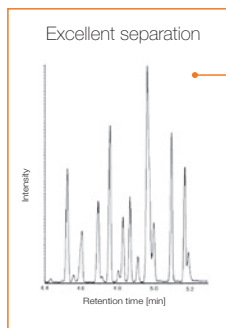
Simple analytical conditions

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™ GCx-plus 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 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.

High-throughput analysis - FastGC



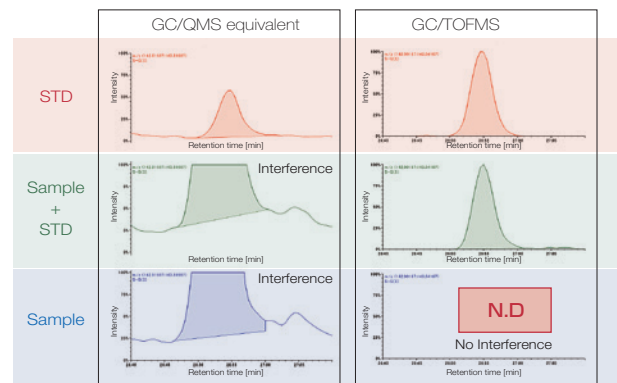
These chromatograms show the presence of 100 pesticide components. In the Fast GC analysis (top), the system acquired data while maintaining chromatographic separation in less than 1/4 of the time needed for the conventional analysis (bottom). The 50 spectra/second high-speed data acquisition system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



Is a time-of-flight mass spectrometer suitable for quantitative analysis?

AccuTOF GCx-plus with a high performance digitizer achieves a wide dynamic range and high reproducibility. AccuTOF™ GCx-plus with high sensitivity, high reproducibility, high qualitative analysis capability, and high throughput will be a major player for the analysis of agrochemical residues in foods.

Extracted Ion Current Chromatograms (EICC) of pesticides in carrot extract



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.

Limit of Quantitation (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.



Application 6

Metabolites

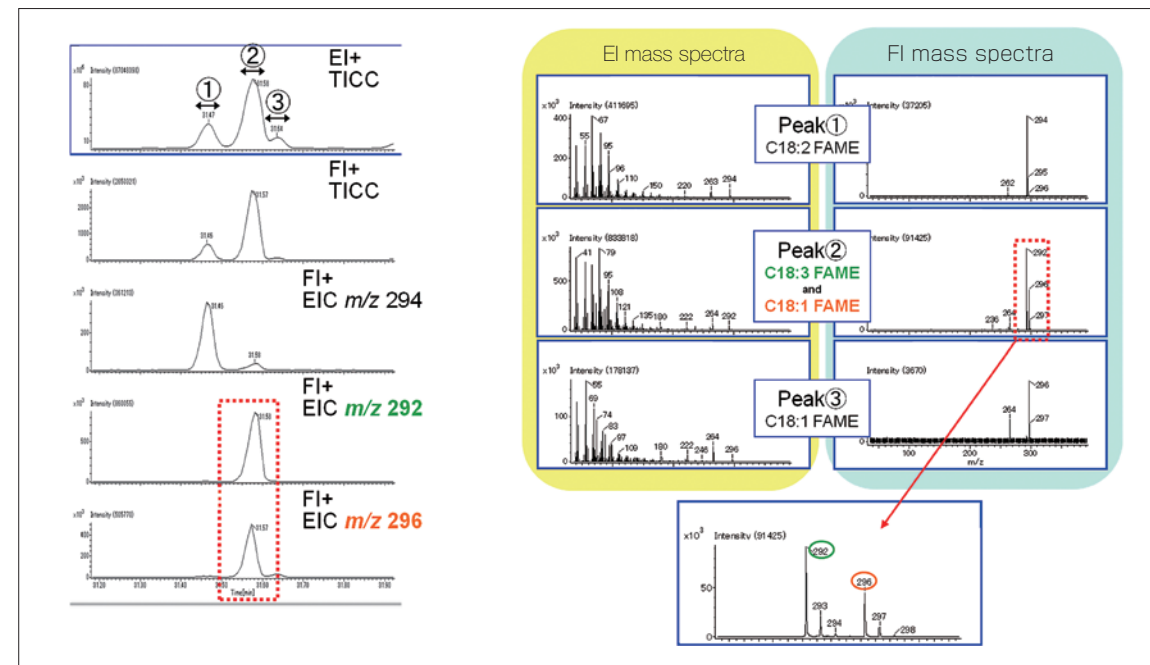


Differentiation of structural isomers and co-eluting analytes with FI

Co-eluting homologues, such as homologous fatty acid methyl esters, can be differentiated with FI as abundant molecular ions and minimal fragmentation. Structural isomers of disaccharides can be differentiated with FI as abundant molecular ions and structurally informative fragment ions.

1. Analysis of fatty acid methyl esters (FAMES)

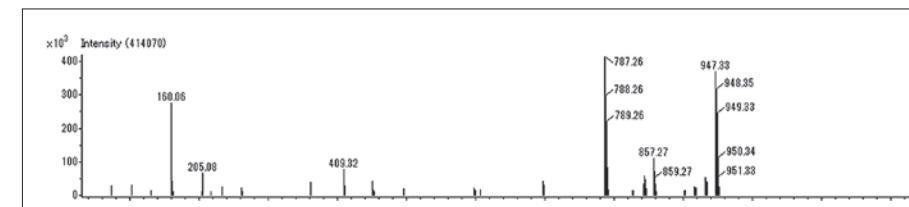
With EI, it was difficult to discern C18:3 FAME and C18:1 FAME as they have nearly identical retention times. With FI, it was easy to recognize both as there were minimal fragment ions.



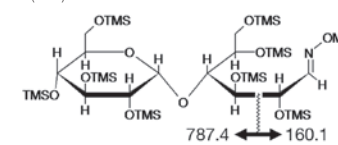
2. Analysis of isomeric disaccharides*

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.

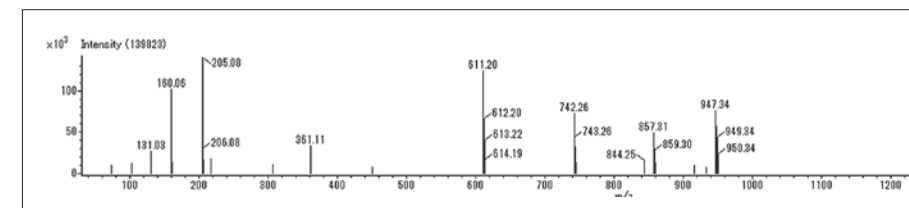
FI mass spectrum of the methyloxime-TMS derivative of maltose



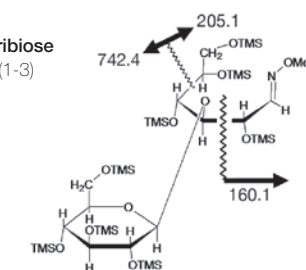
Maltose
Glu-Glu (1-4)



FI mass spectrum of the methyloxime-TMS derivative of laminaribiose



Laminaribiose
Glu-Glu (1-3)



* Furuhashi, T. & Okuda, K. Critical Rev. Anal. Chem., 1 - 16, doi:10.1080/10408347.2017.1320215 (2017).

FAME samples and TMS derivatives of disaccharides courtesy of Dr. Takeshi Furuhashi, Anicom Specialty Medical Institute Inc.



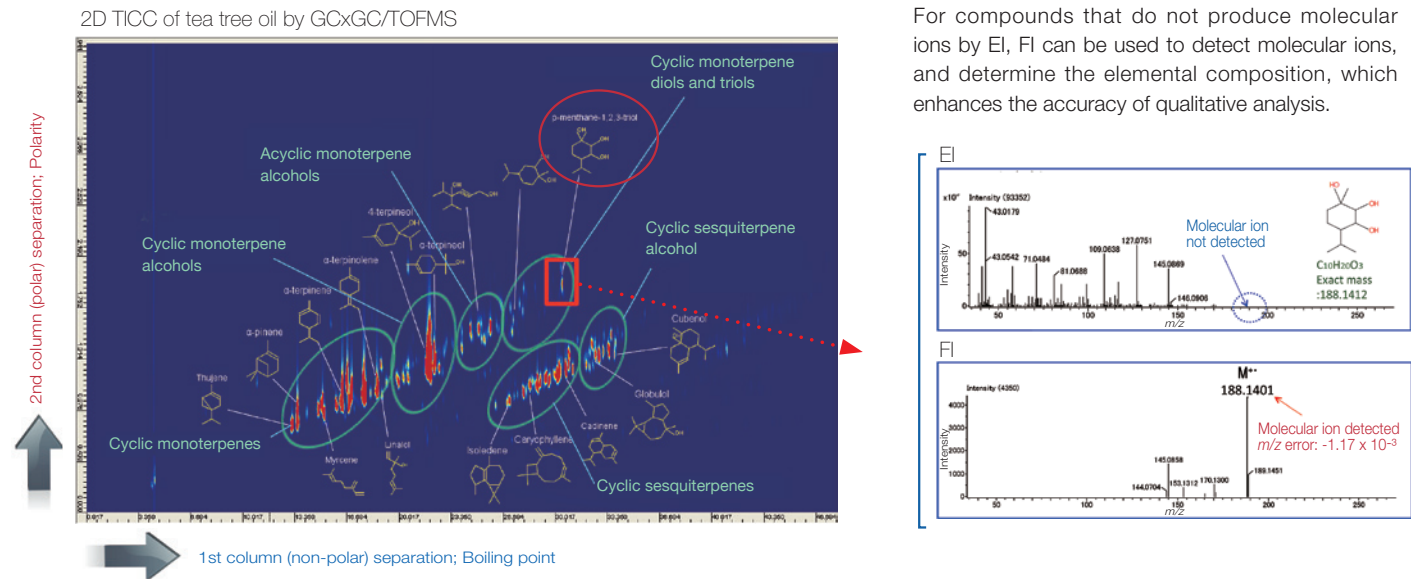
Application 7
Fragrances

Visualization, grouping, and non-target analysis

GCxGC can separate complex mixtures that cannot be separated by ordinary GC. Components that are at trace levels but contribute significantly to sample properties can be found and identified. With mass spectral library searches and accurate mass measurements, separated components can be reliably identified.

1. GCxGC/TOFMS analysis of tea tree oil

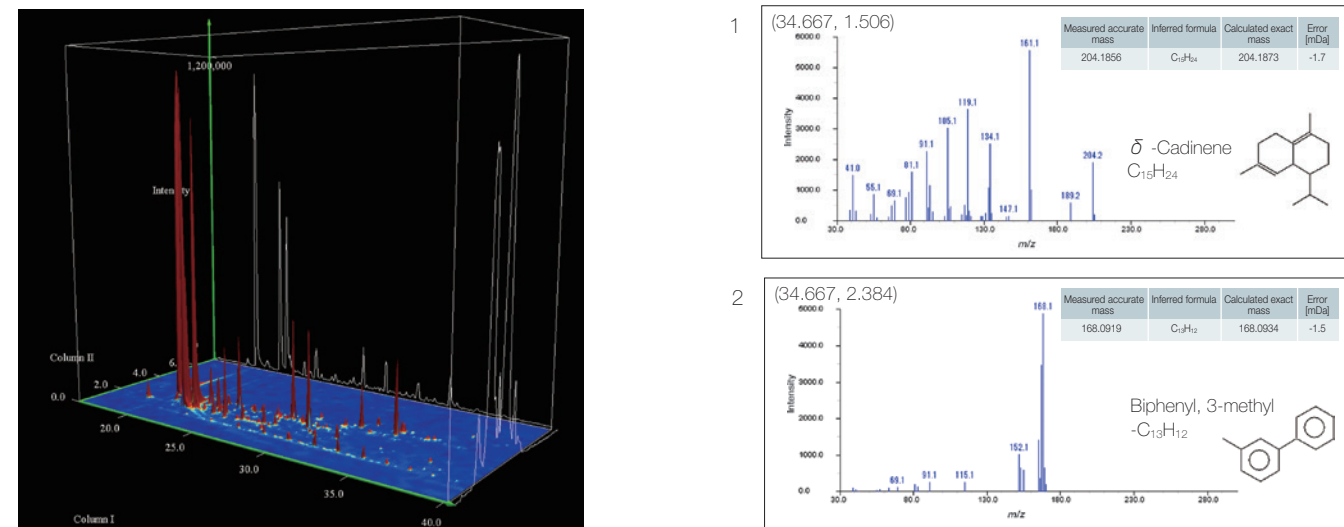
The compounds in an aroma oil were fully separated for grouping. The data offers a visual representation of the complex aroma oil composition.



2. GCxGC/TOFMS analysis of rose oil

Components that cannot be separated by an ordinary 1D GC were separated, detected, and identified.

3D TICC map of rose oil by GCxGC/TOFMS



* ZOEX GCxGC system used for measurement GCxGC chromatogram created by ZOEX GC Image software



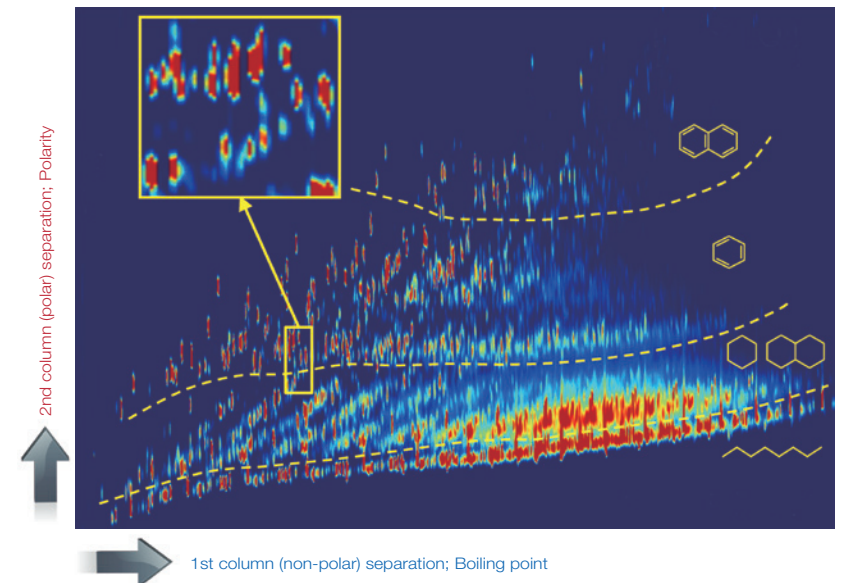
Application 8
Petroleum Products

1. Ultrahigh separation analysis of diesel fuel (GCxGC/TOFMS analysis)

Exact mass measurements are easily accomplished for GCxGC analysis. By combining high resolution with GCxGC, the system can qualitatively analyze trace components.

* ZOEX GCxGC system used for measurement
GCxGC chromatogram created by ZOEX GC Image software

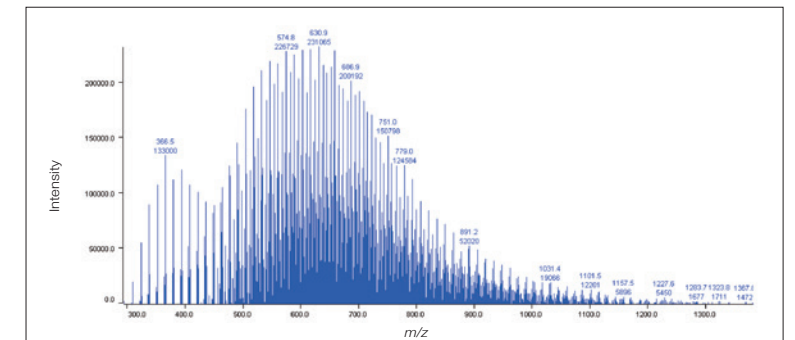
2-dimensional (2D) TICC of diesel fuel by GCxGC/TOFMS



2. Type analysis of microcrystalline wax (MS Tips No. 100)

Type analysis makes it easy to obtain the average molecular weight, molecular weight distribution, and the content of hydrocarbons having different degrees of unsaturation.

FD mass spectrum of microcrystalline wax



Group-type analysis of microcrystalline wax

Series Label	Mn	Mw	Mz	PD	DPn	DPw	DPz	Percent Series	Percent Spectrum
Total / Average	657.0	686.9	718.9	1.0	40.1	42.2	44.5	100.0	64.1
S1	C ₂₇ H _{2n+2}	571.1	617.3	665.3	1.1	33.6	36.9	17.3	11.1
S2	C ₂₇ H _{2n}	529.7	655.0	680.8	1.0	37.9	39.7	24.2	15.5
S3	C ₂₇ H _{2n-2}	670.5	692.3	715.6	1.0	41.0	42.5	13.1	8.4
S4	C ₂₇ H _{2n-4}	715.6	739.0	764.7	1.0	44.3	46.0	8.4	5.4
S5	C ₂₇ H _{2n-6}	688.3	717.9	751.1	1.0	42.5	44.7	22.5	14.5
S6	C ₂₇ H _{2n-8}	710.0	739.6	772.8	1.0	44.2	46.3	14.5	9.3

Mn : Number average molecular weight
Mw : Weight average molecular weight
Mz : Z average molecular weight
PD : Polydispersity index
DPn : Number average degree of polymerization
DPw : Weight average degree of polymerization
DPz : Z average degree of polymerization

FI and FD for the analysis of petroleum products

Petroleum products are highly complex mixtures of hydrocarbons. FI and FD are the only soft ionization techniques universally applicable to various types of hydrocarbons, allowing the determination of molar mass distributions and group-type analysis.

The AccuTOF™ GC series of instruments have been widely accepted in the petroleum industries worldwide.



AccuTOF™ GCx-plus



AccuTOF™ GCx-plus

+ autosampler



AccuTOF™ GCx-plus

+ autosampler

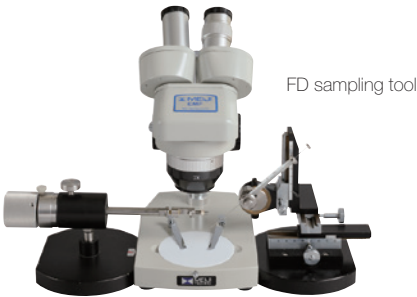
+ direct probe

Standard configuration


Ion source	Electron ionization
Analyzer	Reflectron time-of-flight mass analyzer
Ion detector	Dual microchannel plate
Data acquisition system	Continuous averager
Vacuum system	2 turbo molecular pumps, 2 rotary pumps
Gas chromatograph	Agilent 7890B
Data system	Personal computer, LCD monitor, laser printer, rewritable DVD drive, Windows®operating system, data system software (msAxel)

Optional attachments

- Direct insertion probe
- Direct exposure probe
- EI/FI/FD combination ion source
- FD/FI combination ion source
- EI/PI combination ion source
- CI ion source
- FD sampling tool



Windows is either a registered trademark or a trademark of Microsoft Corporation in the United States and/or other countries.



► Easy linkage to various optional software

- ▷ NIST mass spectral library
- ▷ Escrime for batch quantitative analysis of multiple components
- ▷ Polymerix¹ for analysis of polymers/ hydrocarbon types
- ▷ GC Image² for GCxGC analysis

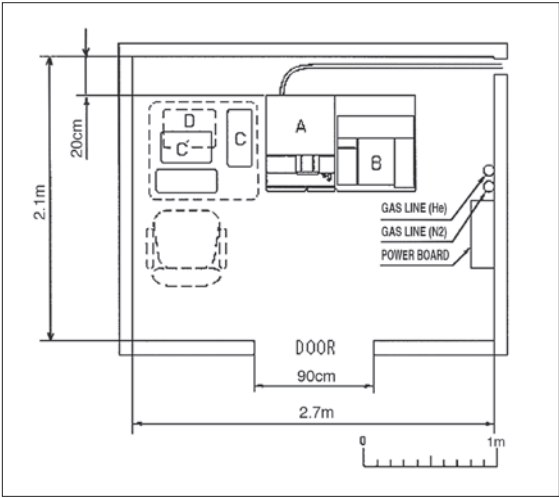
* 1:Sierra Analytics. Inc. * 2 :GC Image. LLC

Installation requirements

Power supply		Installation room	
Main console	Single phase AC190- 210V or 220– 240V, 20A, 50-60Hz	Varying magnetic field	1×10 ⁻⁶ T or less
Gas chromatograph	Single phase, AC 200V or 220V or 230V or 240V, 20 A	Static magnetic field	5×10 ⁻⁴ T or less
Data system	AC100-120V, 15A, 50-60Hz AC200-240V, 7.5A, 50-60Hz	Floor vibration	Amplitude (p-p) 25µm or less, acceleration 0.1m/s ² or less
Grounding	100 Ω 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	Ventilation facility for rotary pump exhaust is required
Gas			
Nitrogen gas			
For purging ion source	0.5 to 0.6 MPa, 97% or better purity		
and analyzer For driving valves			
Helium gas			
For gas chromatograph	0.5 to 0.68MPa, 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.

Example of an installation room



Symbol	Unit	Width mm	Depth mm	Height mm	Weight kg
A	Mass spectrometer	1,172	724	1,224	340
B	Gas chromatograph	582	513	488	49
C	Computer	168	450	456	15
C	TFT LCD monitor	443	220	555	9.2
D	Laser printer	385	279	261	6

- Note
- From the rear of the basic unit of the gas chromatograph, high-temperature air is exhausted. Never place anything behind the unit. 200mm space between rear panel of instrument and wall is neces-sary at least.
 - Exhaust line for rotary pump is required.
 - A table for PC and printer is not included in the standard configuration of AccuTOF™ GCx-plus.

*Specifications subject to change without prior notice.

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