



Scientific / Metrology Instruments
GC-MS integrated qualitative analysis software

Solutions for Innovation

msFineAnalysis series Data Analysis Software

Designed specifically for JMS-Q1600GC, JMS-TQ4000GC, JMS-T2000GC

Auto-analysis software for data acquired by electron ionization/soft ionization



JEOL Ltd.

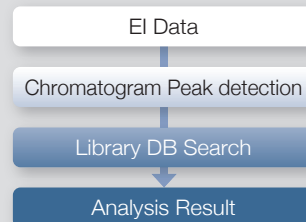
msFineAnalysis series software for automatic

~ You no longer have to only rely on library DB searches for qualitative analysis!

The msFineAnalysis series is an automatic qualitative analysis software that enables **"integrated analysis"** by "📦 **msFineAnalysis iQ**" is designed for low resolution integer mass data analysis, and "📦 **msFineAnalysis**" is and improves work efficiency.



Conventional Analysis Workflow



Problems for

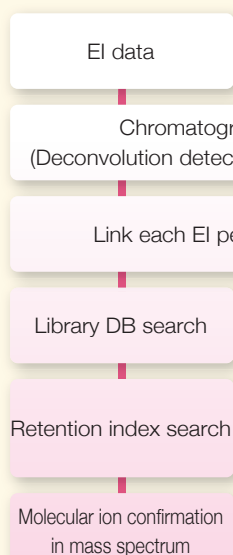
- ① Library DB search re
- ② Unregistered compo
- ③ More sophisticated



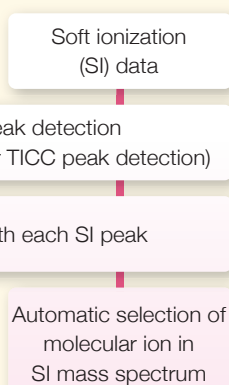
Solutions offered by msFineAnalysis series

Integrated analysis workflow for msFineAnalysis series

Library DB search



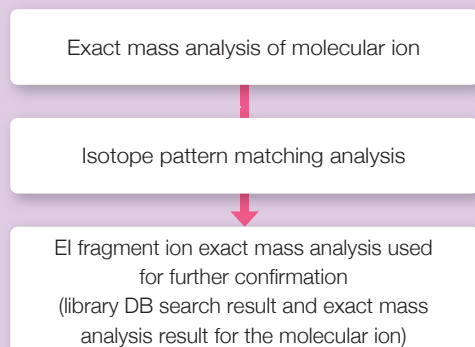
Molecular ion search



Integrated analysis result

- 1) Quickly narrows down candidates by integrated analysis by combining EI data and soft ionization (SI) data.
- 2) Identifies compounds that are not registered in the library DB by exact mass analysis (function only available with 📦 msFineAnalysis)
- 3) After the data is selected, only a single-click is required to generate the automatic integrated report.

Workflow of Exact Mass Analysis of msFineAnalysis



integrated qualitative analysis of GC-MS data

This software adds a new concept that combines EI and soft ionization data~

combining the library database (DB) search using EI data and molecular weight confirmation using soft ionization data. designed for high resolution exact mass data analysis. Each package improves analysis accuracy, shortens work hours,

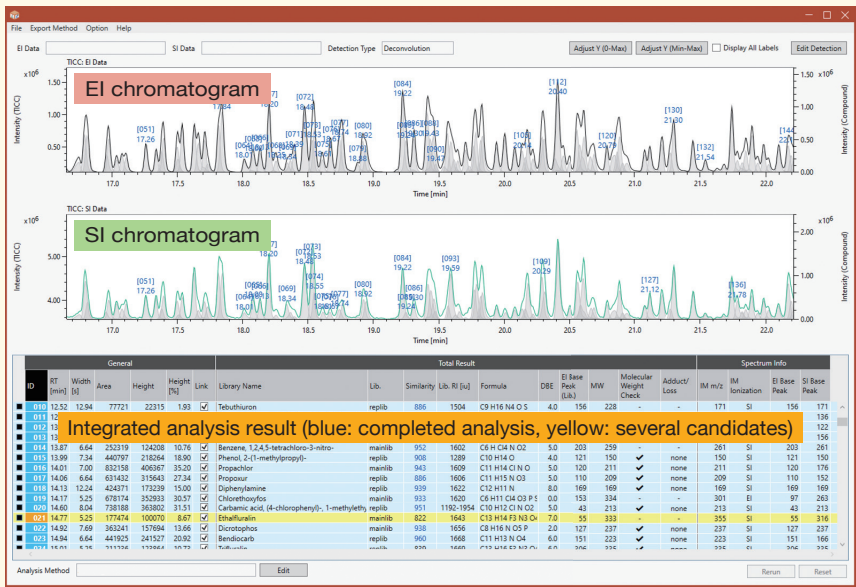
Conventional Qualitative Analysis

- results produce multiple similar candidates, not a single candidate.
- compounds cannot be identified by library DB search.
- analyses take time.



Integrated Analysis Result Window

In the Integrated Analysis Result window, the user confirms the results for the integrated analysis. This window shows the EI and soft ionization (SI) chromatograms, chromatogram information, spectrum information, library DB search, and molecular ion analysis results. When the user double-clicks the desired line in the analysis result list, a separate mass spectrum analysis window appears that allows the user to confirm the search result and molecular ion analysis result. The user can also update the results or perform the analysis again. Additionally, **msFineAnalysis**, which can analyze exact mass data, can also suggest the correct molecular formula for components that are not registered in the library database and provide partial structural information from the EI data as well.



Chromatogram information Integrated analysis result (library DB search + molecular ion confirmation) Spectrum information

Full Functionality of the msFineAnalysis Series

Two Sample Comparison Function (Differential Analysis)



The two sample comparison function uses reproducibility of the p-value on the vertical axis and a volcano plot which indicates the intensity ratio between two samples on the horizontal axis. This information enables a visual confirmation of the differing components between two samples. For example, it is possible to confirm the component that increases or decreases by comparing the reference product and defective product, or to confirm the components that are characteristic in a new material by comparing it with an existing material.

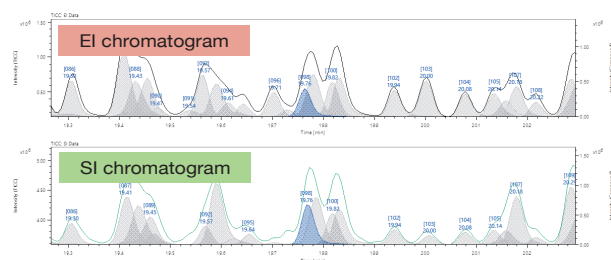
After differential analysis between samples, the normal msFineAnalysis integrated analysis is performed for all components. For a two sample comparison function, it is possible to set n=1, 3, 5, for the number of measurements for each sample. In the case of n=1, it is not possible to evaluate the statistical reproducibility. However, it is possible to confirm which components are different. This function allows the user to do sample comparisons even when it is not possible to acquire more than one measurement for each sample.



Deconvolution Detection



Deconvolution detection can detect trace components that may not be obvious in the TICC as a result of several component peaks overlapping and/or coelute as a single peak. As a result, it is not necessary to create an extracted ion chromatogram (EIC) one-by-one manually, as was previously necessary.



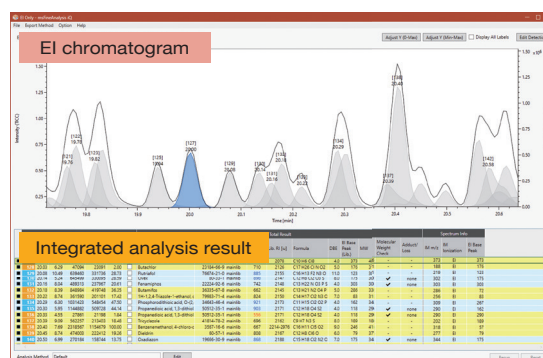
EI: black solid line: TICC, gray peaks: deconvolution peak (blue: currently selected)

SI: green solid line: TICC, gray peaks: deconvolution peak (blue: currently selected)

Analysis by EI Data Alone



Analysis using EI data alone is also possible. When soft ionization sample data is not available, msFineAnalysis can produce an integrated analysis report in which the EI data is used for both the library DB search and the molecular ion search.





Function of msFineAnalysis iQ



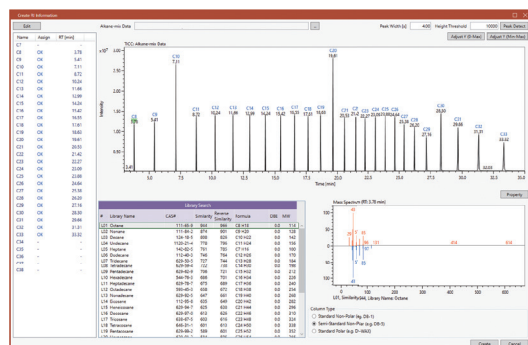
Function of msFineAnalysis

Retention Index Qualitative Analysis



Retention index (RI) is a relative index value based on the retention time (RT) of an n-alkane standard mixture. This qualitative analysis function is performed by converting the retention time of the target component into a retention index and then comparing it with the retention index value in the database, etc.

With the msFineAnalysis series, it is possible to narrow down the qualitative analysis result further by using the retention index.



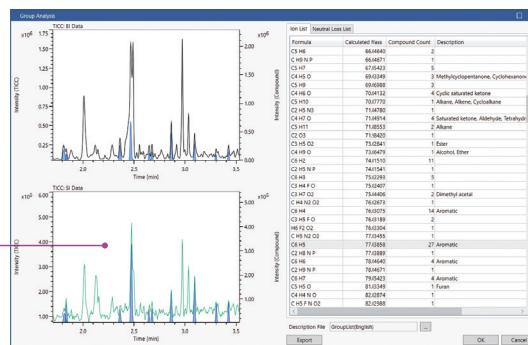
Retention index creation screen:

GC/El data of n-alkane mixture

Group Analysis



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



Extracted components containing a specified ion or neutral loss

Group analysis screen

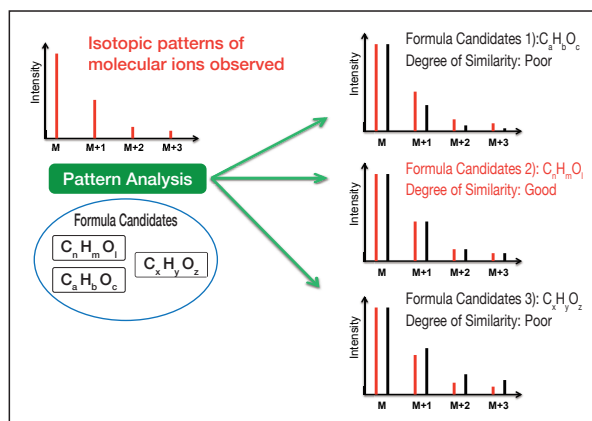
Specifying an observed ion or neutral loss

The operator can review analytical results of certain compound groups quickly and exclusively by using, for example, C_6H_5 fragment ions specific to aromatic compounds or Br fragment ions specific to bromine compounds.

Isotope Pattern Analysis of Molecular Ions



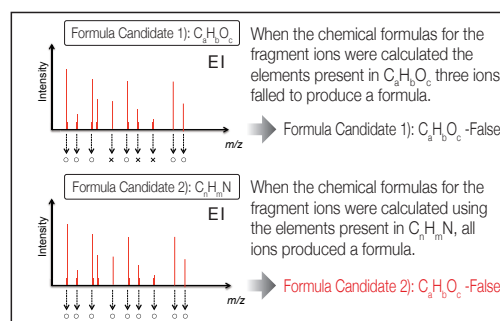
Multiple formula candidates often appear during molecular ion exact mass analysis. When this happens, it is possible to filter the formula candidates by isotopic pattern analysis.



Exact Mass Analysis of Fragment Ions



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



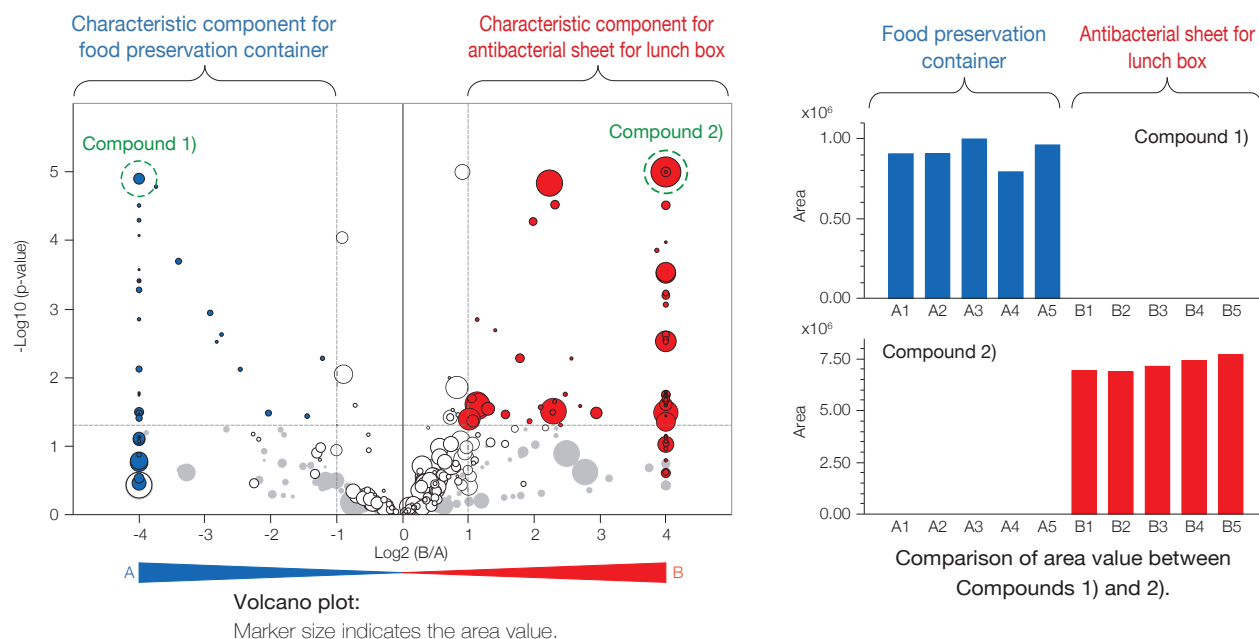
Analysis of Additives in Commercial Polypropylene Products by Py/GC/QMS

Polypropylene (PP) is used in a variety of products such as tableware, stationery, electrical appliances, films, sheets, and scientific laboratory equipment due to its low cost and good heat and chemical resistance. These PP products will have different additives based on the intended use or application. In this example, we compare the resulting measurements of two commercial PP products: a food preservation container and an antibacterial sheet for use in lunch boxes. Pyrolysis GC/QMS (Py/GC/QMS) was used for the sample measurements, and the data was analyzed by using msFineAnalysis iQ.

•Differential Analysis Results

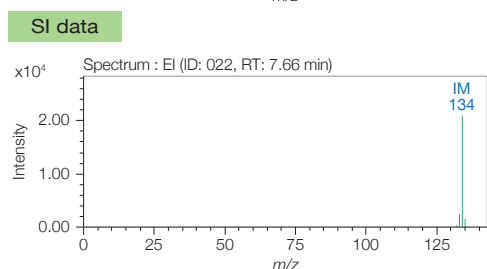
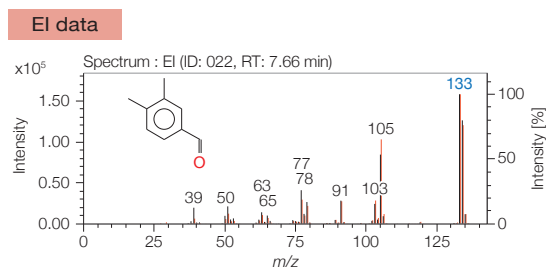
The differential analysis results using msFineAnalysis iQ are shown in the lower left figure. The characteristic components for each sample are visualized as the plot, thus allowing easy confirmation of the components that is different in each sample.

Additionally, we specified the components with the best reproducibility and the strongest intensity ratio between the two samples as compounds 1) and 2), and confirmed their area values. It was found that each component was only detected in one of the two samples, respectively.

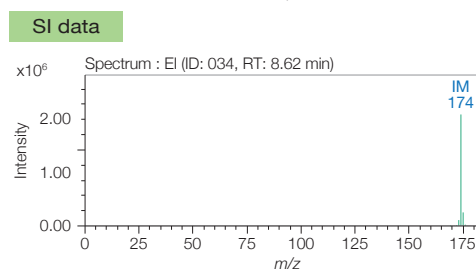
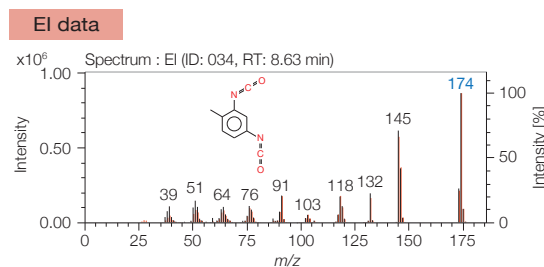


•Integrated Analysis Results

As a result of integrated analysis of compounds 1) and 2), compound 1) was identified as “3,4-Dimethylbenzaldehyde” and compound 2) was identified as “2,4-Tolylene diisocyanate”. 3,4-Dimethylbenzaldehyde is a material used to make resins transparent. 2,4-Tolylene diisocyanate is a raw material for polyurethane, indicating that polyurethane is contained in the antibacterial sheet for lunch boxes. The msFineAnalysis iQ software makes it possible to easily perform an extraction of differing components as well as produce a qualitative analysis report for these components.



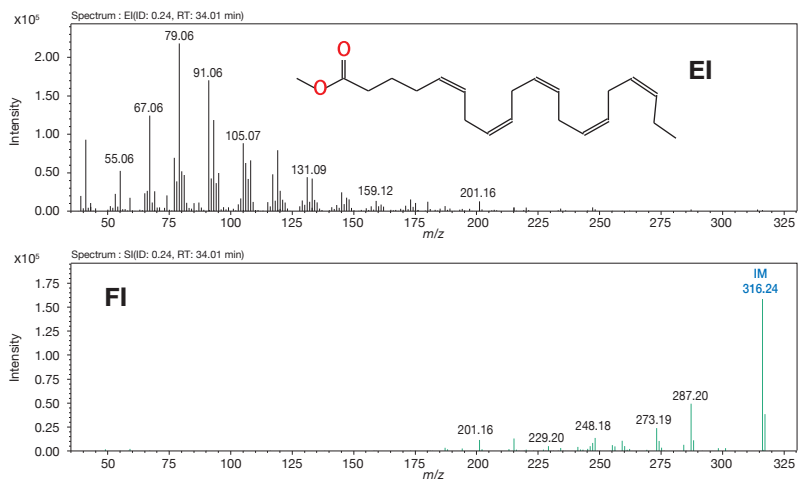
Mass spectra of compound 1)



Mass spectra of compound 2)

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

The composition of fatty acids in fats and oils (triacylglycerol) can be obtained by hydrolyzing the fats and oils, derivatizing the resulting fatty acids into methyl esters, and measuring them by GC-MS. Polyunsaturated fatty acids such as eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA), are important components in biochemistry, but their methyl esters are known to have molecular ions that cannot be detected by using EI. However, Field Ionization (FI) is ideal for the measurement of polyunsaturated FAMES.



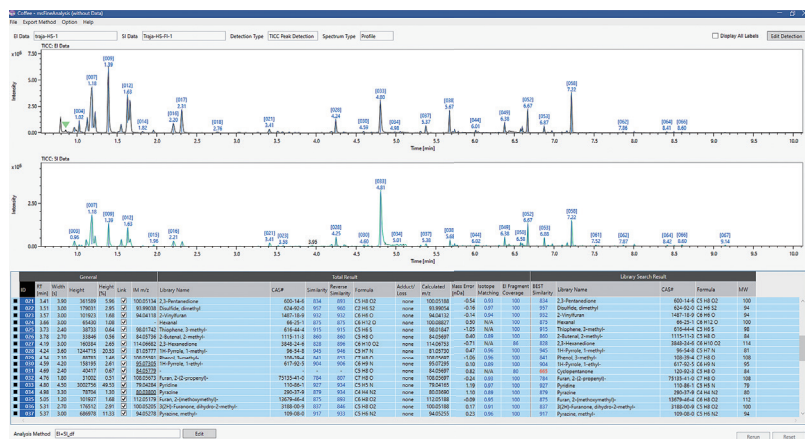
Mass spectra of EPA methyl ester

[illegible]

Integrated analysis results of 37-component FAMES

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






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



Integrated analysis result of coffee aroma components

A commercial 37-component FAME standard mixture (Restek, 200-600 ng/uL) was measured for this example. Molecular ions were confirmed in the FI mass spectra for all components measured. A molecular ion was detected as the base peak in each FI mass spectrum even for EPA methyl esters which have 5 double-bonds in their alkyl group.

Therefore, it is possible to fully complement the library DB search results with the exact mass analysis results for FAMES. Consequently, the msFineAnalysis integrated analysis allowed us to determine the composition formula for all components.

	 msFineAnalysis iQ	 msFineAnalysis
Applicable instrument	 Gas Chromatograph Quadrupole Mass Spectrometer JMS-Q1600GC UltraQuad™ SQ-Zeta  Gas Chromatograph Triple Quadrupole Mass Spectrometer JMS-TQ4000GC UltraQuad™ TQ <div> Available ionization methods <ul style="list-style-type: none"> · EI (Electron Ionization) · PI (Photoionization) · Low energy EI · CI (Chemical Ionization) </div>	 Gas Chromatograph Time-of-Flight Mass Spectrometer JMS-T2000GC AccuTOF™ GC-Alpha <div> Available ionization methods <ul style="list-style-type: none"> · EI (Electron Ionization) · FI (Field Ionization) · PI (Photoionization) · Low energy EI · CI (Chemical Ionization) </div>
Integrated analysis using data from EI/SI methods	<input type="radio"/>	<input type="radio"/>
Analysis using EI method data alone	<input type="radio"/>	<input type="radio"/>
Deconvolution detection	<input type="radio"/>	<input type="radio"/>
Library DB search	<input type="radio"/>	<input type="radio"/>
Retention index qualitative analysis	<input type="radio"/>	<input type="radio"/>
Confirmation of molecular ions	<input type="radio"/>	<input type="radio"/>
Two sample comparison (differential analysis)	<input type="radio"/>	<input type="radio"/>
Exact mass analysis	<input checked="" type="checkbox"/>	<input type="radio"/>
Isotope pattern matching of composition formula candidates	<input checked="" type="checkbox"/>	<input type="radio"/>
Group analysis	<input checked="" type="checkbox"/>	<input type="radio"/>

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