JEOL

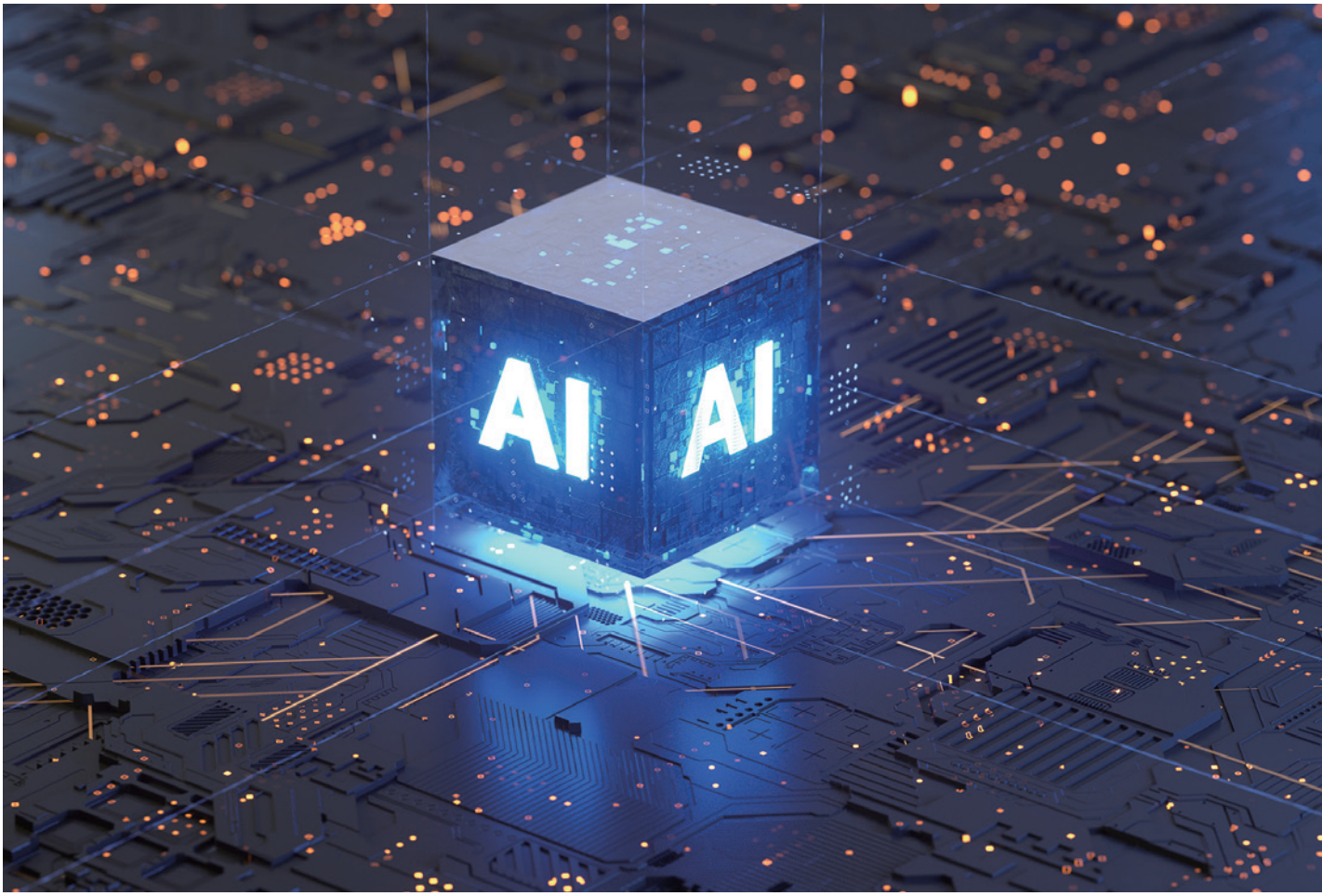
Scientific / Metrology Instruments

Unknown Compounds Structure Analysis Software

Solutions for Innovation

msFineAnalysis AI

Automatic structure analysis software for data acquired by electron ionization and soft ionization
Designed specifically for GC-HRTOFMS: JMS-T2000GC AccuTOF™ GC-Alpha



JEOL Ltd.

Advanced AI technologies enable structure analysis of unknown compounds

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

P.9

Retention Index Qualitative Analysis

#3

P.10

Differential Analysis

#4

#1

AI Structure Analysis

P.3-8

Group Analysis
- Fragment Ions
- Additives
- Off-flavor Components

#2

Deconvolution Detection

P.9

Integrated Analysis
- EI/Soft Ionization Data Automatic Analysis

Library Database Search
- EI Mass Spectrum Database Search

Analysis Using EI Method Data Alone
- Molecular Ion Search in EI Mass Spectrum

EI Fragment Ion Analysis
- Accurate Mass Analysis

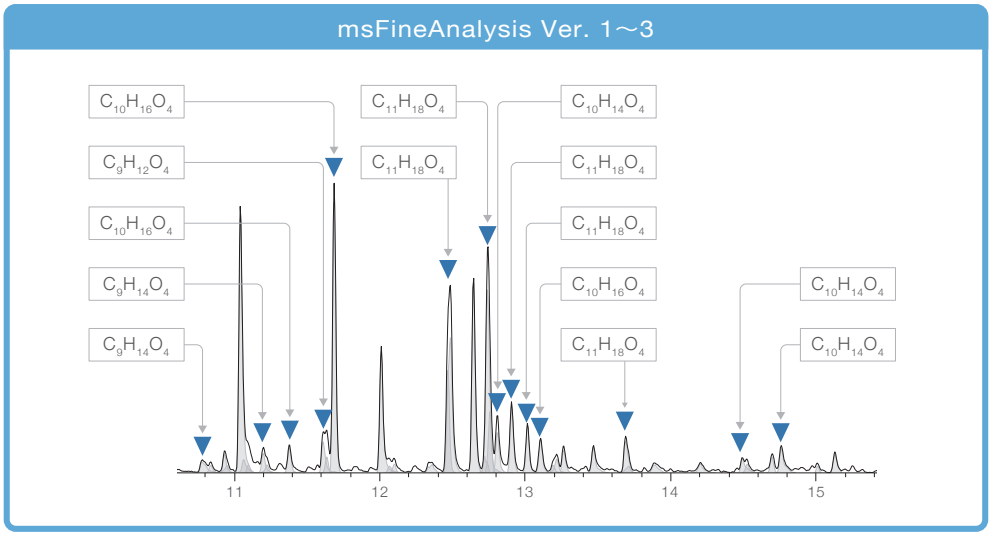
Isotopic Pattern Analysis
- Molecular Formula Search
- M/M+H Correction

#1 AI Structure Analysis

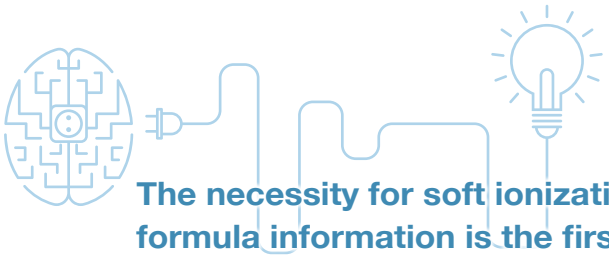
Evolving innovative solutions:
From molecular formula estimation to structural formula prediction for unknown compounds

For an unknown compound that is not registered in a library database (▼), the conventional msFineAnalysis algorithms automatically suggest a molecular formula. To take it a step further, msFineAnalysis AI enables automatic prediction of structures for all detected components.

Image of analysis results in the previous generation msFineAnalysis



Change by AI Structural Analysis



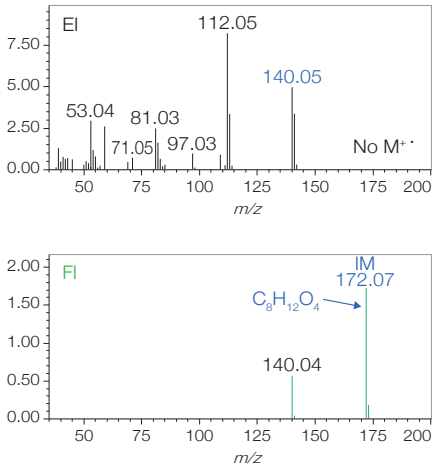
The necessity for soft ionization: Reliable acquisition of molecular formula information is the first step in structure analysis!

EI mass spectral data is used for library databases so EI methods are widely used for qualitative analysis of GC-MS samples. However, since EI is a hard ionization method, many fragment ions are observed, and in many cases, it is not uncommon to observe minimal or no signal for the molecular ions.

Additionally, for unknown substances not registered in the library databases, it is difficult to distinguish, using the EI mass spectra alone, whether the largest observed *m/z* is actually the molecular ion or just a fragment ion. In these cases, a soft ionization method is an effective tool for determining this information.

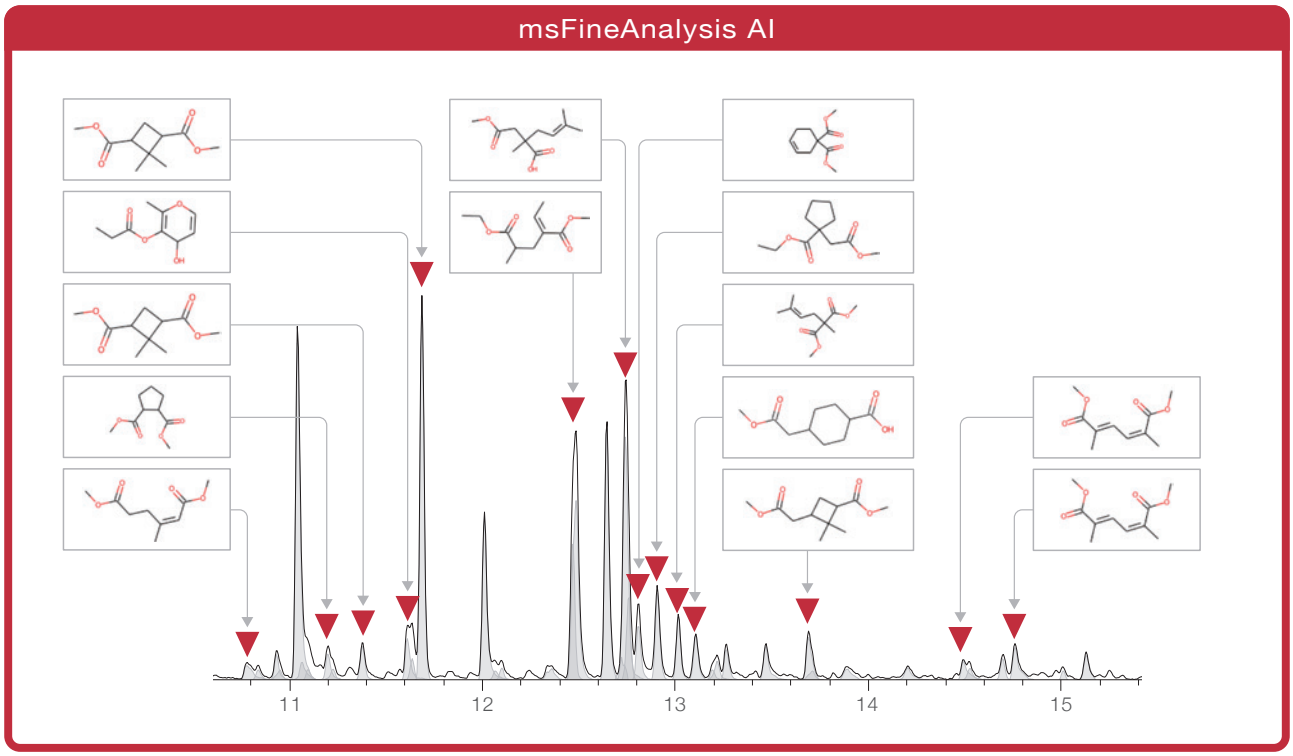
With the AccuTOF™ GC-Alpha, a variety of soft ionization methods including FI, PI, and CI are optionally available with the system. These techniques can assist in distinguishing ions (e.g. molecular ions and protonated molecules) that provide molecular weight information that then makes it possible to accurately determine the molecular formula information for unknown components.

Since molecular formula information is an important starting point for AI structure analysis, soft ionization is critically important for identifying unknown compounds.

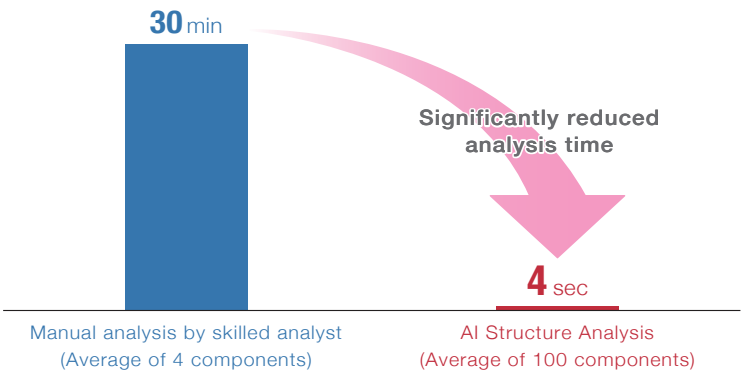


Mass spectrum of component not registered in library

Image of analysis results in msFineAnalysis AI

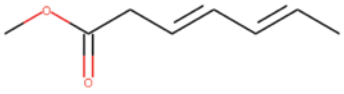


Manual Structure Analysis by Skilled Analyst vs. AI Automatic Structure Analysis



※Measured with JMS-T2000GC standard configuration PC

The time required for structure analysis was compared for the compounds observed in an acrylic resin measured by Py-GC-TOFMS and were not registered in the NIST library database.
Even an analyst with more than 30 years mass spectrometry experience required **approximately 2 hours for structure analysis of 4 components**, which is 30 minutes per component. On the other hand, AI structure analysis completed **100 components in less than 7 minutes**, which is 4 seconds per component.



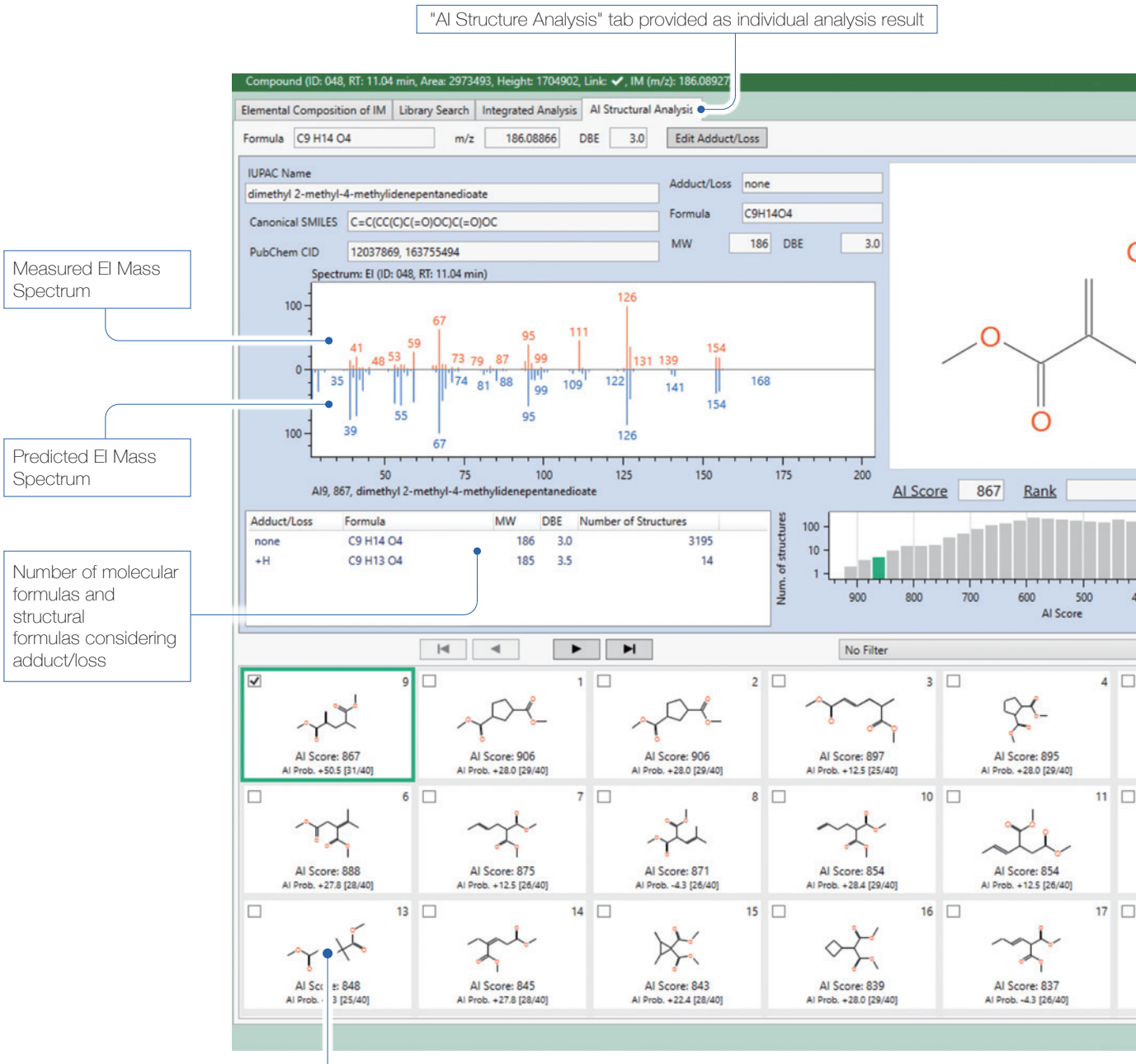
AI Score: 779

AI structure analysis score (similarity) between the structural formula estimated by a skilled analyst and the correct structural formula, indicating that the structural formula is predicted with good similarity.

#1 AI Structure Analysis

Automatic Structure Analysis Using Two AIs:
Stable structure analysis without the need for an online environment

msFineAnalysis AI offers an automated structure analysis function.
Based on the structural formula information of more than 100 million organic compounds recognized in the world and calculations using two newly developed AI models, it provides candidate structural formulas even for components that are not registered in the library database.



Structural Formula Prediction by **Main AI**

Determine a structural formula using mass spectra predicted from **100 million compounds**

- Displays ranked structural formulas in list.
- Selecting a structural formula updates the information that is displayed.
- Below each structural formula is an AI score that indicates the match percentage between structural formula and mass spectrum.

Partial Structure Prediction by **Support AI**

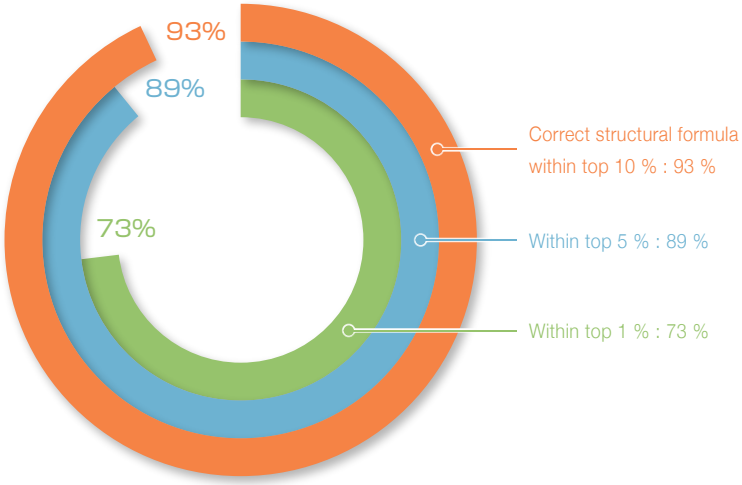
Assist in interpreting analysis result by **predicting partial structures** from the measured mass spectrum.

- Displays the predicted partial structure information
- Partial structure predicted and present are on the left, predicted and absent are on the right.
- Those with a blue background are the partial structures that match the selected structural formulas. Those with a red background are those that do not match.

#1 AI Structure Analysis

AI Structure Analysis **Prediction Accuracy**

The NIST20 library database is used by the Main AI employed in AI structure analysis for learning and evaluation. The prediction accuracy tests confirmed that the correct structure was in the top 1% for 73% of the compounds, and in the top 10% for 93% of the compounds.

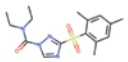
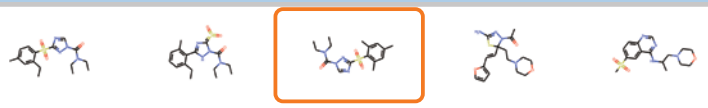
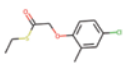
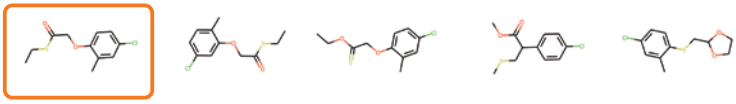
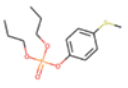
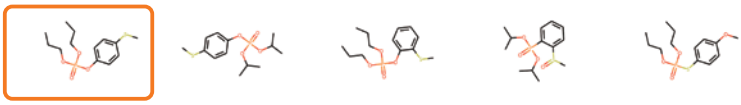
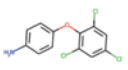
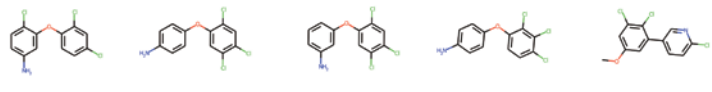
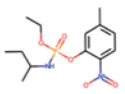
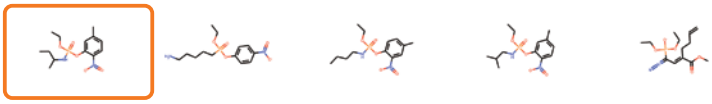
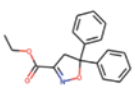
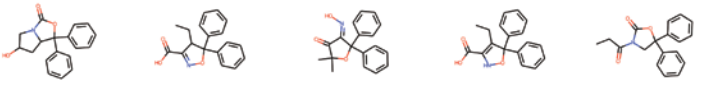


Correct structural formula ranking in 14681 compounds

Structures with the same composition formula as the target compounds (14581 compounds) are prepared from PubChem. The rank order of the correct structure is verified among them.

Of the 14581 compounds verified, the correct structure was obtained within top 1% rank order in 73% (10644 compounds).

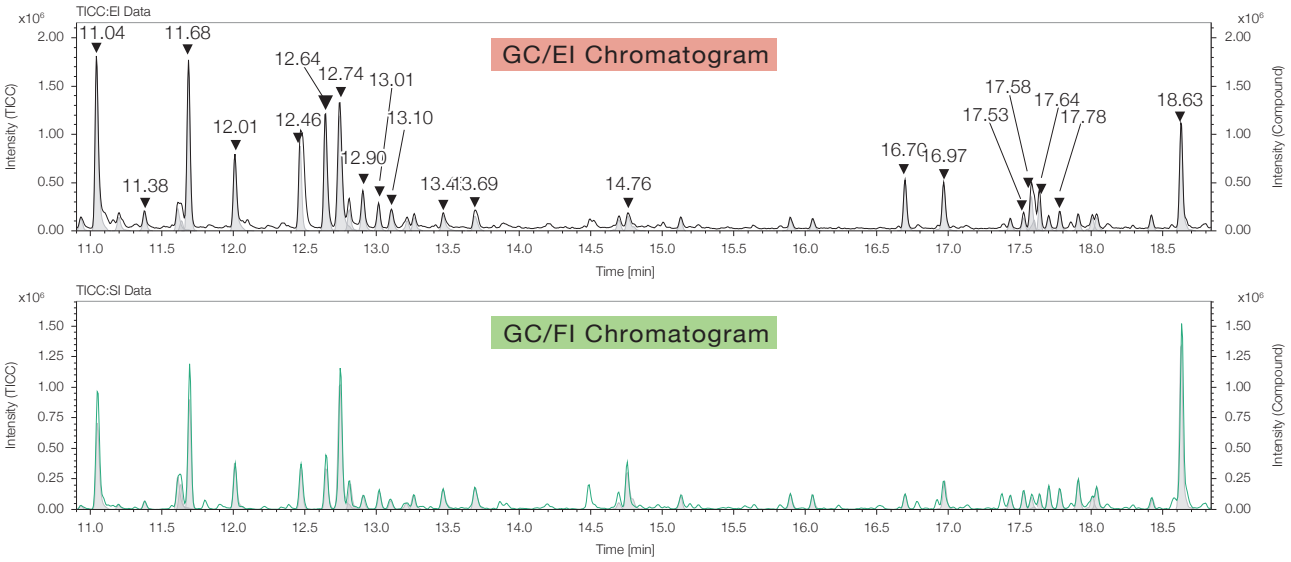
Subsequently, 6 known compounds that were not registered in the NIST20 library database were analyzed, and the correct structure was ranked highest for three compounds. For the remaining compounds, the top structures listed in the structure analysis results all shared similar features with the correct formula.

Compound Name	Correct Structure	AI Score	Rank Order (Total Candidates)	Top 5 Structural Formulas
Cafenstrole		741	3 (2933)	
MCPA-thioethyl		735	1 (729)	
Propaphos		802	1 (27)	
CNP-amino		710	14 (618)	
Butamifos oxon		675	1 (56)	
Isoxadifen-ethyl		586	22 (5348)	

: Correct structure

AI Structure Analysis **Application**

The AI structure analysis results for an acrylic resin measured by Py-GC-HRTOFMS are shown below. For the 20 compounds that had structures that could not be confirmed with the NIST20 library database, AI structure analysis was performed after determining their molecular formula through integrated analysis.



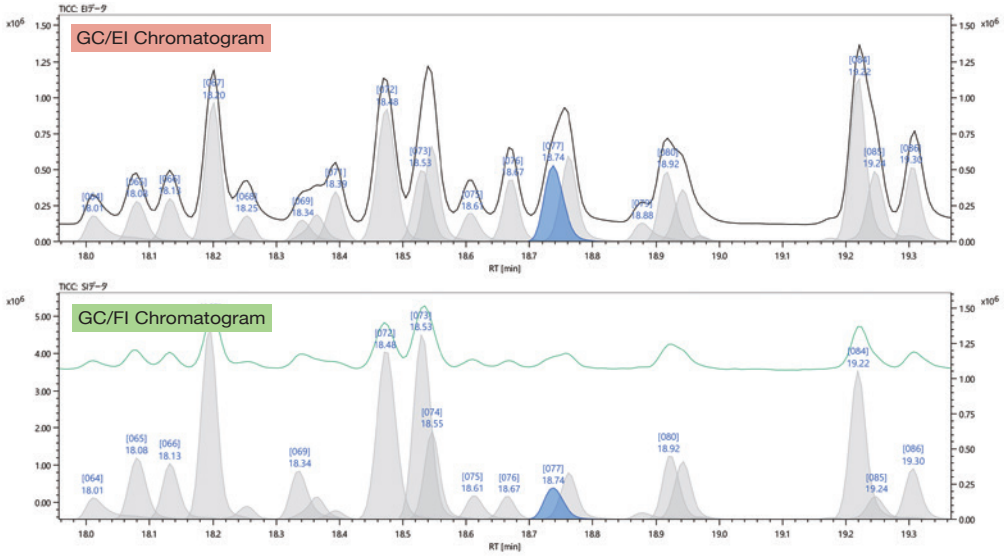
All of these compounds had structures that included methyl esters (reflecting the acrylic resin monomer structure) shown for the higher ranked possibilities. This information allowed us to estimate that all of the compounds targeted for structure analysis are acrylic resin thermal decomposition products.

RT	Composition Formula	Top 5 Structural Formulas
11.04	C9 H14 O4	
11.38	C10 H16 O4	
11.68	C10 H16 O4	
12.01	C9 H14 O4	
12.46	C10 H16 O4	
12.64	C10 H16 O4	
12.74	C11 H18 O4	
12.90	C11 H18 O4	
13.01	C11 H18 O4	
13.10	C11 H18 O4	

RT	Composition Formula	Top 5 Structural Formulas
13.46	C10 H14 O4	
13.69	C11 H18 O4	
14.76	C10 H14 O4	
16.70	C13 H20 O6	
16.97	C13 H20 O6	
17.53	C14 H22 O6	
17.58	C13 H20 O6	
17.64	C14 H22 O6	
17.78	C14 H22 O6	
18.63	C15 H24 O6	

#2 Deconvolution Detection

Chromatographic peak deconvolution can detect trace components that may not be obvious in the TICC due to the coelution of several components.

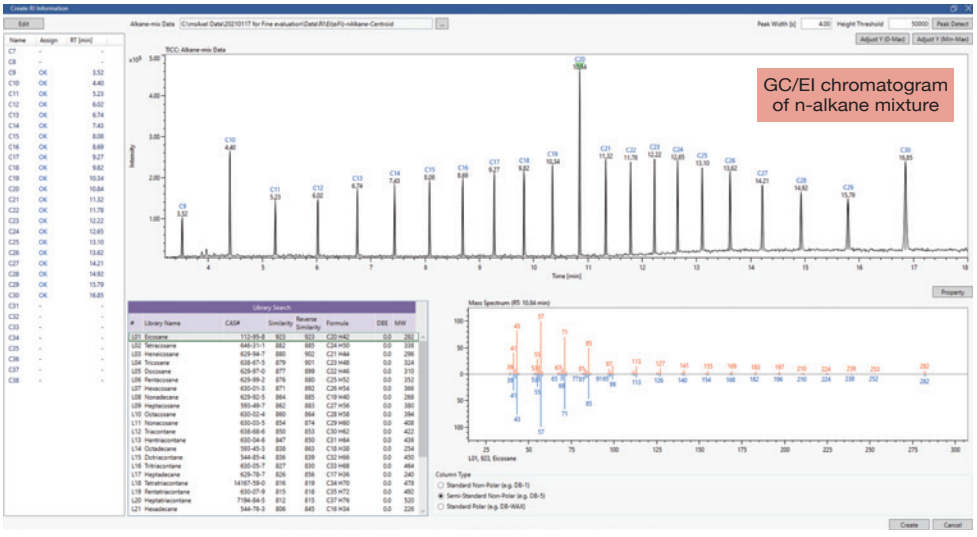


EI: black solid line: TICC, gray peaks: deconvolution peak (blue: currently selected)
FI: green solid line: TICC, gray peaks: deconvolution peak (blue: currently selected)

This step simplifies the data analysis process by defining which ions go with each compound and eliminates the need for creating extracted ion chromatograms (EICs).

#3 Retention Index Qualitative Analysis

Retention index (RI) is a relative index value based on the retention times (RT) for an n-alkane standard mixture.

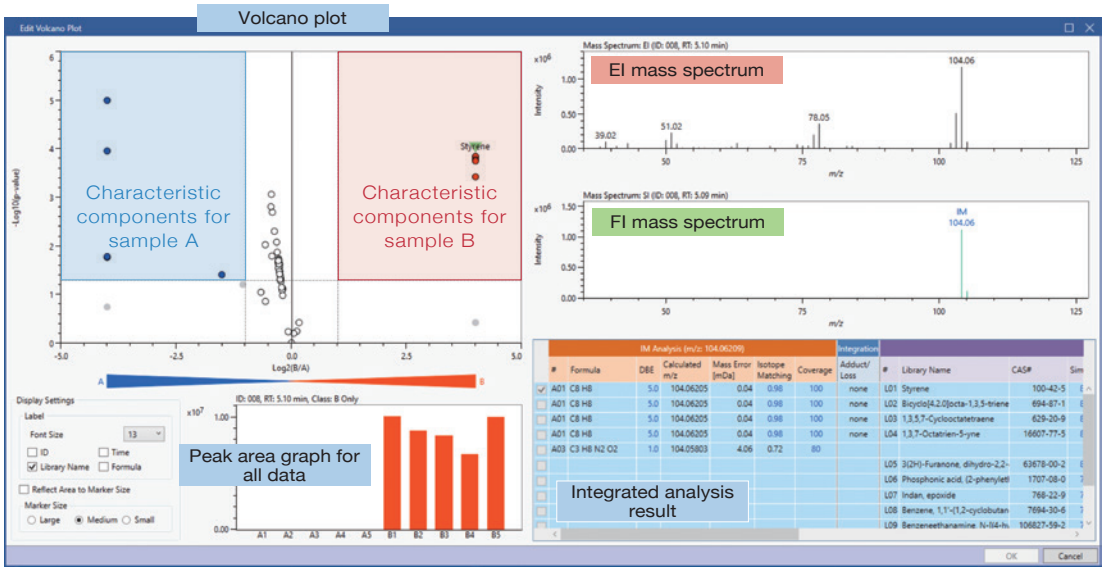


Retention Index Creation Screen

This qualitative analysis function is performed by converting the RT of the target component into a RI and then comparing it with the RI value listed in the databases, etc. With msFineAnalysis AI, it is possible to narrow down the qualitative analysis result further by using the RI.

#4 Differential Analysis · **Two Sample Comparison**

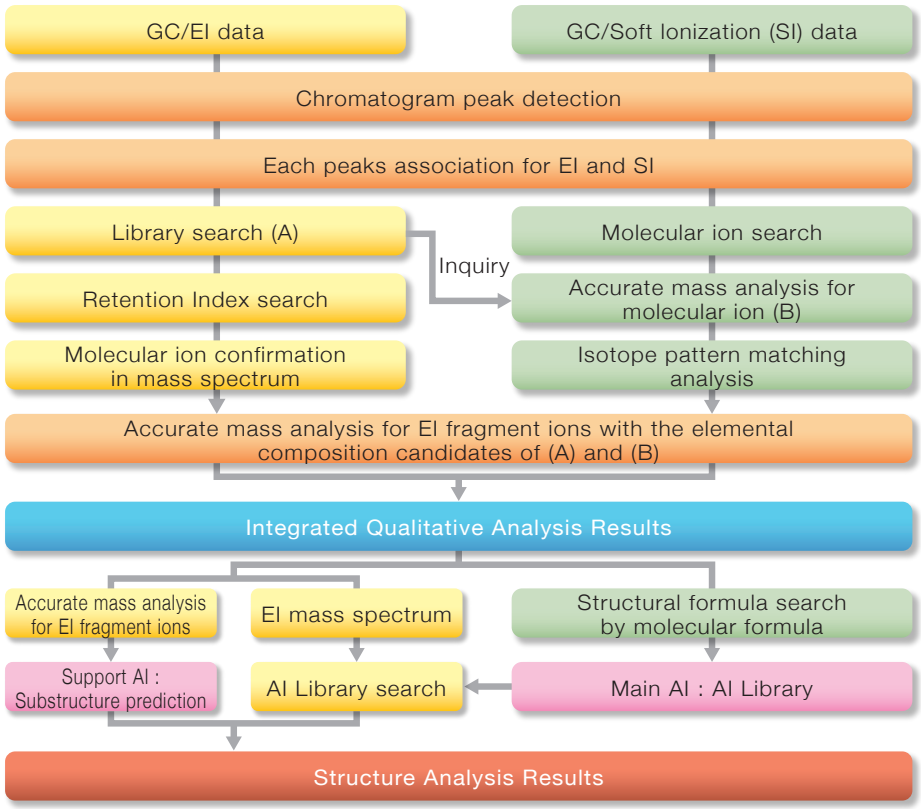
This function uses the reproducibility of the p-value on the vertical axis and a volcano plot which indicates the intensity ratio between two samples on the horizontal axis.



Detailed analysis – Volcano plot
(A: Reference product, B: Defective product)

This information enables a visual confirmation of the differing components between two samples. For example, it is possible to confirm if a component increases or decreases when comparing a reference product to a defective product or to identify characteristic components in a new material by comparing it to an existing material. For a two sample comparison, it is possible to set n=1, 3, 5 for the number of measurements for each sample.

msFineAnalysis AI Analysis Flow



Major Specifications

JMS-T2000GC AccuTOF™ GC-Alpha	
Mass Resolution	30,000@*m/z* 614
Mass Accuracy	1 ppm@EI standard ion source
Mass Range	*m/z* 4-6,000
Ionization Methods	EI、CI、PI、FI、FD、DEI、DCI

msFineAnalysis AI	
Specifications	· Automatically detecting peaks and creating mass spectra · Creating mass spectra by manual peak detection · Creating mass spectra by deconvolution processing · Analyzing identical components of two measurement data items · Analyzing molecular ions according to two mass spectra · Variance component analysis · Displaying analysis results using retention indices · Displaying NIST database search results · Displaying exact mass calculation results · Displaying isotope pattern analysis results · Displaying measurement conditions · User interface: English · AI Structure analysis

JEOL Ltd.
3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577
www.jeol.com ISO 9001・ISO 14001 Certified

▼ Local office

• AUSTRALIA & NEW ZEALAND • BELGIUM • BRAZIL • CANADA • CHINA • EGYPT • FRANCE • GERMANY • GREAT BRITAIN & IRELAND • INDIA • ITALY • KOREA • MALAYSIA • MEXICO • RUSSIA • SCANDINAVIA • SINGAPORE • TAIWAN • THAILAND • THE NETHERLANDS • UAE (Dubai) • USA

No.2151L209C(Bn)