

## Effect of high mass accuracy on the analysis result by JMS-T2000GC — Effect to narrow down the result of msFineAnalysis integrated analysis —

Related Product: Mass Spectrometer(MS)

### Introduction

JEOL Ltd. recently announced the JMS-T2000GC “AccuTOF™ GC-Alpha” which is the 6<sup>th</sup> generation GC high resolution time-of-flight MS (GC-HRTOFMS) in the “AccuTOF™ GC” series that was first released in 2004. The GC-Alpha (Fig. 1) represents a significant improvement in capabilities over the previous model with three times higher mass resolving power (10,000→30,000 @  $m/z$  614) and three times higher mass accuracy (3ppm→1ppm, EI standard ion source). In this work, we used the thermal decomposition of an acrylic resin to evaluate how improved mass accuracy can affect the analysis results for a complex sample. Additionally, the msFineAnalysis Version 3 software included with the JMS-T2000GC was used to quickly determine the impact of improved mass accuracy on the qualitative analysis results.

### Experimental

Table 1 shows the measurement conditions for the pyrolysis GC-MS measurements. A JMS-T2000GC equipped with a Frontier Lab pyrolyzer and the JEOL EI/FI combination ion source was used for the measurements, and a commercially available acrylic resin was used as the sample -- 0.2mg for EI method and 1.0mg for FI method, respectively. The resulting data was then analyzed by using the msFineAnalysis integrated workflow (next section, Fig. 2) to examine the effects of high mass accuracy on the analysis results.

**Table 1. Measurement and analysis conditions**

Pyrolysis conditions		MS conditions	
Pyrolyzer	EGA/PY-3030D(Frontier Lab)	Spectrometer	JMS-T2000GC (JEOL Ltd.)
Pyrolysis Temperature	600°C	Ion Source	EI/FI combination ion source
GC conditions		Ionization	EI+:70eV, 300µA FI+:-10kV, 40mA/30msec
Gas Chromatograph	8890A GC (Agilent Technologies)	Mass Range	$m/z$ 35-800
Column	ZB-5MSi (Phenomenex) 30m x 0.25mm, 0.25µm	Data processing condition	
Oven Temperature	40°C(2min)-10°C/min -320°C(15min)	Software	msFineAnalysis (JEOL Ltd.)
Injection Mode	Split mode (100:1)	Library database	NIST17
Carrier flow	He:1.0mL/min	Tolerance	±5mDa, ±2mDa



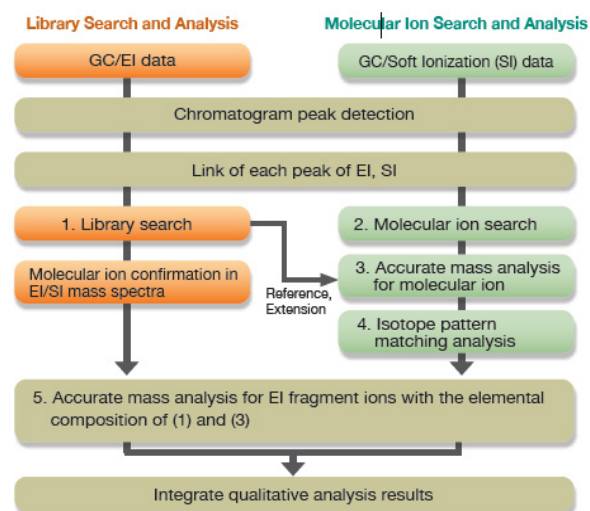
**Fig. 1 JEOL GC/HR-TOFMS systems: JMS-T2000GC**

### msFineAnalysis Software

Fig. 2 shows the msFineAnalysis workflow in which GC/EI data and GC/soft ionization (SI) data are analyzed together to automatically produce an integrated qualitative analysis report. The 5 qualitative analysis steps that are automatically executed are:

1. Library database search using EI mass spectrum
2. Automatic search of molecular ion in the SI mass spectrum
3. Accurate mass analysis for the molecular ion
4. Isotope pattern matching analysis to narrow down the candidate molecular formulas
5. Accurate mass analysis of EI fragment ion and narrowing down molecular formula candidates by using the composition condition of molecular formula candidate obtained in 1 and 4.

By combining the accurate mass analysis of the EI and SI mass spectra, msFineAnalysis cannot only identify components registered in the library but can also determine the elemental composition for unregistered components.

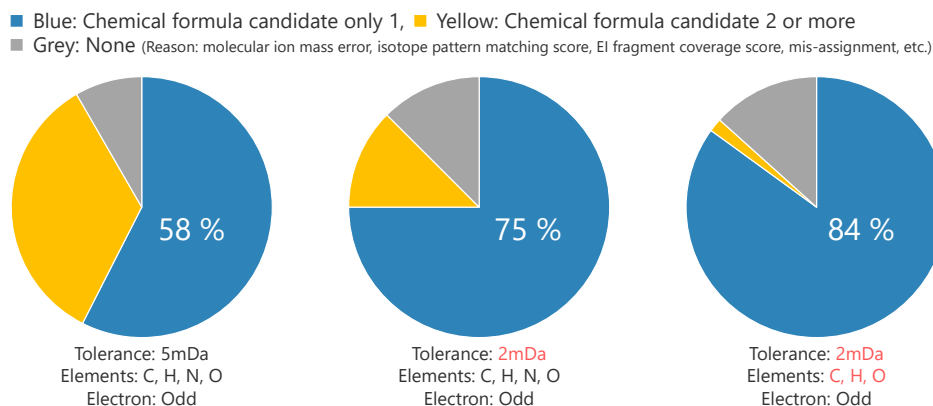


**Fig. 2 msFineAnalysis workflow**

## Result

For accurate mass analysis, an error tolerance is specified based on the mass accuracy capabilities of the instrument. The previous generation models (i.e. JMS-T200GC) required an error tolerance of  $\pm 5$  mDa for the elemental compositions. However, with the higher mass accuracy of the JMS-T2000GC, it is possible to narrow this error tolerance, which in turn lowers the number of possible elemental compositions calculated for each analyte. The goal of these experiments was to examine the effect of error tolerance for the 120 components (Intensity  $\geq 0.05\%$ ) that were observed during thermal decomposition of the acrylic resin.

Fig. 3 shows the results for the automatic analysis for the pyrolysis of acrylic resin using msFineAnalysis. The blue color shows the percentage of components that resulted in one molecular formula candidate, the yellow shows the percentage that had two or more molecular formula candidates, and the gray shows the percentage with no clear molecular formula candidate. The left pie chart shows the analysis results when using an error tolerance of  $\pm 5$  mDa. Because of this wider tolerance, there were many analytes with more than one candidate molecular formula (yellow). Consequently, only 58% of the 120 components were narrowed down to a single molecular formula candidate. Next, the error tolerance was lowered to  $\pm 2$  mDa, and the results are shown in the Fig.2 central pie chart. The narrower tolerance eliminated many false positive candidates and increased the number of components with only one molecular formula candidate to 75%. Next, the elements used for the elemental composition calculations were narrowed to include only C/H/O because the acrylic resin substructure only includes these elements. The pie chart on the right shows the results of removing nitrogen from the search while continuing to use the narrower tolerance of  $\pm 2$  mDa. As a result, the number of components identified with one molecular formula increased to 84% (101 components).

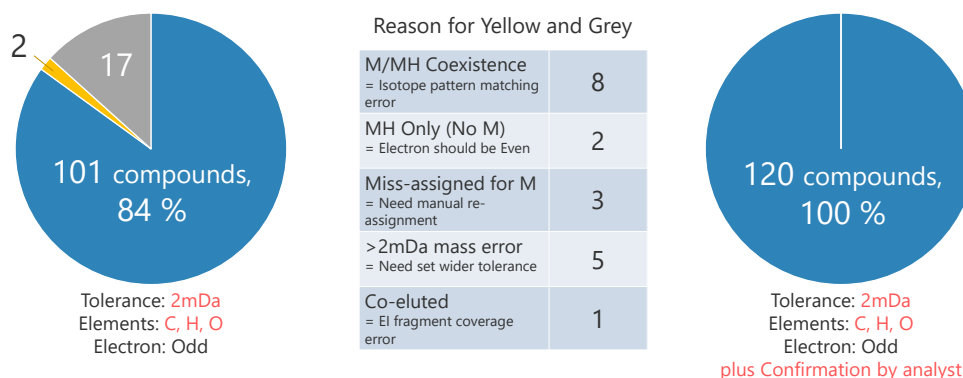


**Fig. 3 Comparison of automatic analysis results for 120 components**

The remaining 19 components were not automatically narrowed down to a single candidate composition for the following reasons:

- $[M]^+$  and  $[M+H]^+$  were present together so the isotope pattern did not match.
- Only  $[M+H]^+$  were observed (since the number of electrons in the proton-added molecule is even, the Odd electron search constraint did not give the correct result).
- The relative intensity of the molecular ion was lower than the default threshold of 10% for ion peak detection and was not correctly assigned.
- The absolute intensity of the molecular ion was low and the peak shape was poor, resulting in a mass error of more than 2mDa.
- It was considered to be a fully co-eluting component, and the EI fragment ion coverage was low.

By manually verifying the measurement data and analysis results for these final 19 components, we were able to narrow down the list to one candidate molecular formula (Fig. 4), thus identifying a single elemental composition for all 120 components that resulted from the pyrolysis of acrylic resin.



**Fig. 4 Confirmation by analyst for 19 components**

## Conclusions

The high mass accuracy of the new JMS-T2000GC allows the analyst to use narrower mass error tolerances within msFineAnalysis. As a result, the software was able to automatically narrow down the number of molecular formula candidates to a single possibility for the majority of the observed components. For components that had more than one candidate formula (yellow) or did not have a formula candidate (gray), the analyst was able to quickly focus on these components and manually verify the mass spectrum and analysis results. The combination of the JMS-T2000GC with the automatic analysis capabilities of the msFineAnalysis software provides a powerful solution that simplifies the qualitative analysis of complex samples.

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