

## Effect of JMS-T2000GC high mass resolution on the analysis result –KMD Plot comparison using msRepeatFinder–

Related Product: Mass Spectrometer(MS)

### Introduction

Recently, JEOL announced the release of the JMS-T2000GC “AccuTOF™ GC-Alpha”, which is the 6th generation GC-HRTOFMS in the JEOL “AccuTOF™ GC” series (Fig. 1). The GC-Alpha achieves 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) than the previous model. In this work, we used direct probe field desorption (FD) of crude oil (a very complex mixture) to monitor the effects of improved resolution. Additionally, the JEOL msRepeatFinder software was used to examine the crude oil data by using Kendrick mass defect (KMD) plots in order to more clearly visualize the effects of improved mass resolution on the analysis results.



Fig. 1 JEOL GC-HRTOFMS systems: JMS-T2000GC

### Experimental

Crude oil from the Gulf of Mexico (SRM2779, NIST) was used as the sample. The previous generation JMS-T200GC and new generation JMS-T2000GC equipped with EI/FI/FD combination ion sources were used for the sample analysis. Table 1 shows the measurement conditions for these systems. The data from each system was then analyzed by using msRepeatFinder to confirm the effect of improved mass-resolving power on the analysis results.

Table 1. Measurement and analysis conditions

MS conditions	
Spectrometer	JMS-T2000GC (JEOL Ltd.) JMS-T200GC (JEOL Ltd.) (Previous model)
Ion Source	EI/FI/FD combination ion source
Ionization	FD+: -10kV, 0→51.2mA/min→50mA
Mass Range	$m/z$ 35-1,600
Data processing condition	
Software	msRepeatFinder (JEOL Ltd.)

## Result

Fig. 2 shows the FD mass spectrum obtained by both instruments. Although the overall spectrum patterns were very similar, a closer inspection of the peaks showed that the peak separation differed significantly for each instrument. The JMS-T2000GC (Fig. 2(a)) showed a clear mass separation of each hydrocarbon component, even in the high mass range above  $m/z$  600, that is the result of the new system having a higher mass resolving power. In contrast, the mass separation for the previous model was insufficient, particularly in the high mass range, to adequately resolve the mass peaks from each other.

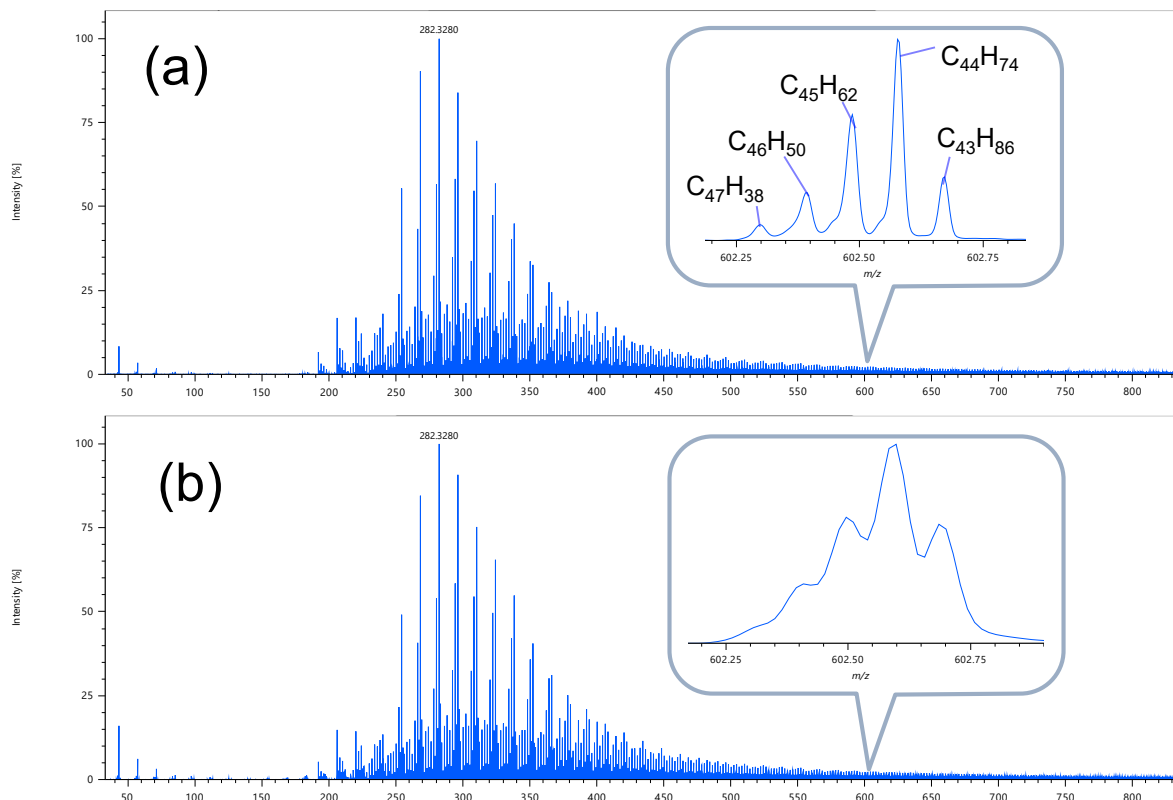


Fig. 2 FD mass spectra for crude oil: (a) JMS-T2000GC data, (b) Previous model data

Next, msRepeatFinder was used to visualize each FD mass spectrum with KMD plots (Fig. 3). The JMS-T2000GC KMD plot (Fig. 3(a)) clearly showed the family of components over the full mass range (including the components above  $m/z$  600). This outcome is a direct result of the improved peak separation, as shown in Fig. 2. On the other hand, the KMD plot for the previous model showed very poor results for the peaks above  $m/z$  600, with many components disappearing because of insufficient mass separation. Basically, the unresolved peaks are being treated as single components despite the fact that there are multiple components, thus resulting in the loss of KMD Plot information in the high mass range.

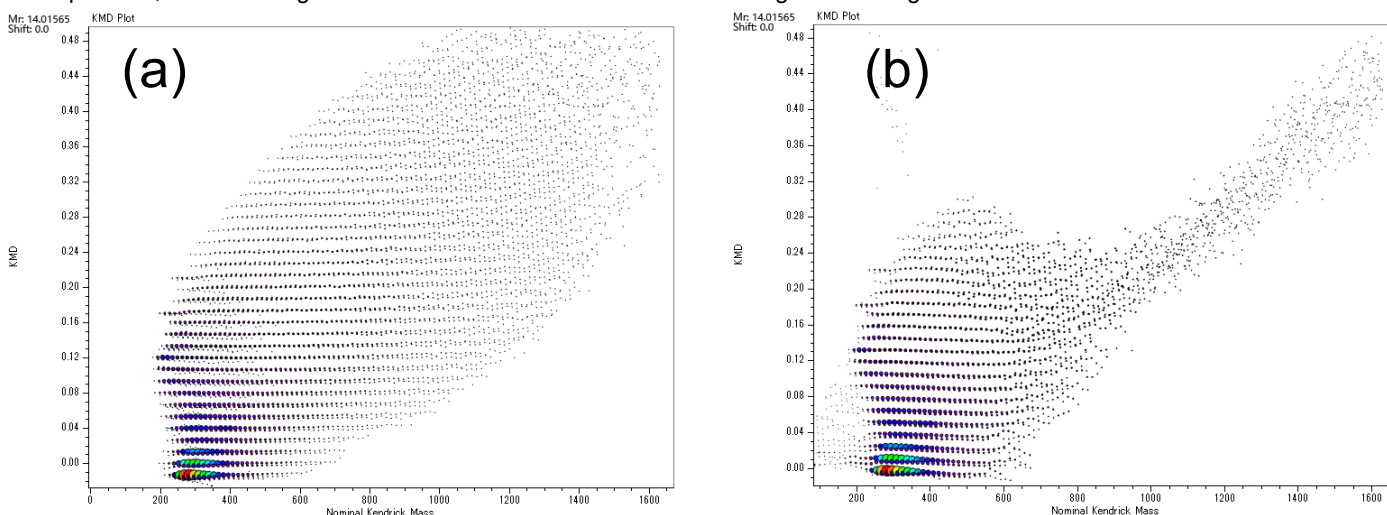


Fig. 3 KMD Plots of FD mass spectrum: (a) JMS-T2000GC data, (b) Previous model data

## Conclusions

The above results confirmed that the high resolving power achieved by the JMS-T2000GC was particularly effective for direct mass measurements (FD probe) of complex materials like crude oil. Additionally, the KMD plots clearly showed that the T2000GC high mass-resolution dramatically increased the number of detected components as a result of the improved mass separation.

Copyright © 2021 JEOL Ltd.

Certain products in this brochure are controlled under the "Foreign Exchange and Foreign Trade Law" of Japan in compliance with international security export control. JEOL Ltd. must provide the Japanese Government with "End-user's Statement of Assurance" and "End-use Certificate" in order to obtain the export license needed for export from Japan. If the product to be exported is in this category, the end user will be asked to fill in these certificate forms.