Structural analysis of 2,2,4-trimethyl-1,3-pentanediol monoisobutyrate using msFineAnalysis AI

Product used: Mass Spectrometer (MS)

Introduction

2,2,4-trimethyl-1,3-pentanediol monoisobutyrate (TMPMB) is used as an adjuvant in adhesives and paints. Furthermore, the amount to use as an alternative plasticizer has increased, since phthalate esters which were used as plasticizers have been restricted by the RoHS Directive. On the other hand, health hazards such as sick house syndrome have been reported due to increased exposure, so the Ministry of Health, Labor and Welfare is considering to restrict it. Thermal desorption (TD)-GC-MS method has been proposed as an analysis method, and an example of analysis using a quadrupole mass spectrometer JMS-Q1600GC was introduced in MSTips No. 435. Figure 1 shows the structural formula of TMPMB. It has two structural isomers, but only one is registered in the NIST library used for qualitative analysis. In this MSTips, we used a time-of-flight mass spectrometer JMS-T2000GC and unknown compounds structure analysis software msFineAnalysis AI to confirm whether the other structural formula could be obtained correctly.

Figure 1 Structure formula of 2,2,4-Trimethyl-1,3-pentanediol monoisobutyrate (TMPMB)

Experiment

Three compounds under consideration to restrict were used as measurement samples, and 100 ng of each were added to a TD tube. Table 1 shows the measurement conditions of TD-GC-MS.

Table 1 Measurement conditions

TD conditions	
Thermal Desorption	TD-100xr (Markes International Ltd)
Sample tube type	Tenax TA
Tube desorption	280°C (10min), 30mL/min, Splitless
Focusing trap type	General purpose Hydrophobic (T2)
Trap cooling	0 °C
Trap desorption	280°C (3min), 2mL/min, Splitless
Flow path temperature	200 °C

GC conditions	
Gas Chromatograph	8890A GC (Agilent Technologies)
Column	ZB-5MSi (Phenomenex) 30m x 0.25mm, 0.25µm
Oven Temperature	40°C(2min)-15°C/min -320°C(10min)
Carrier flow	He, 2.0mL/min
MS conditions	
Spectrometer	JMS-T2000GC (JEOL Ltd.)
Ion source	EI/FI combination
Ionization	EI(70eV), FI
Ion source temperature	250 °C
Mass range	*m/z* 10-800

Results

Figure 2 shows result of msFineAnalysis AI. Qualitative information of all peaks could be obtained by integrated analysis.

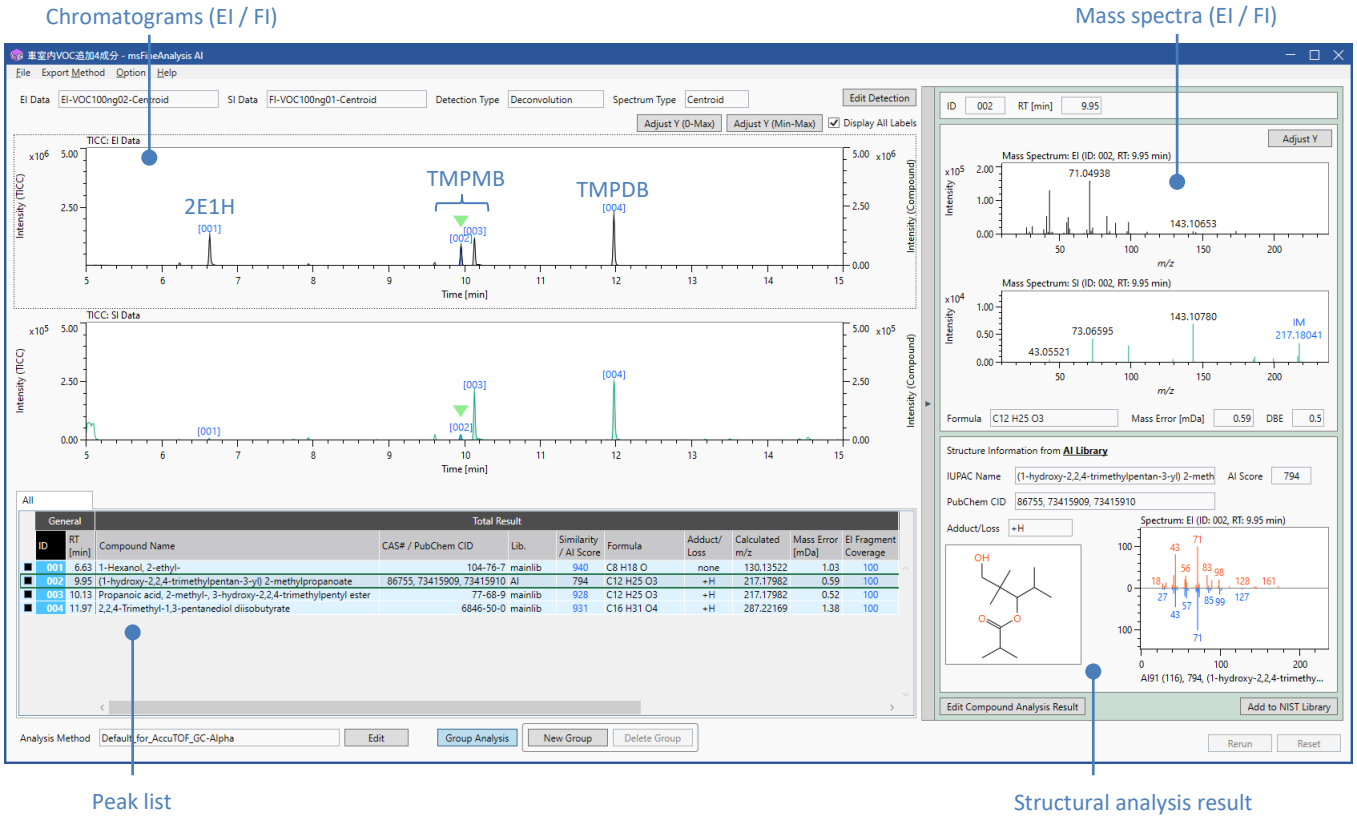

Figure 2 Screen shot of msFineAnalysis AI

Figure 3 shows the structural analysis results of peak ID 002 and ID 003. The structural formula of peak ID 002 which is not registered in NIST library could be correctly obtained. The similarity between the measured mass spectrum and the AI predicted mass spectrum was relatively high with AI score 794.

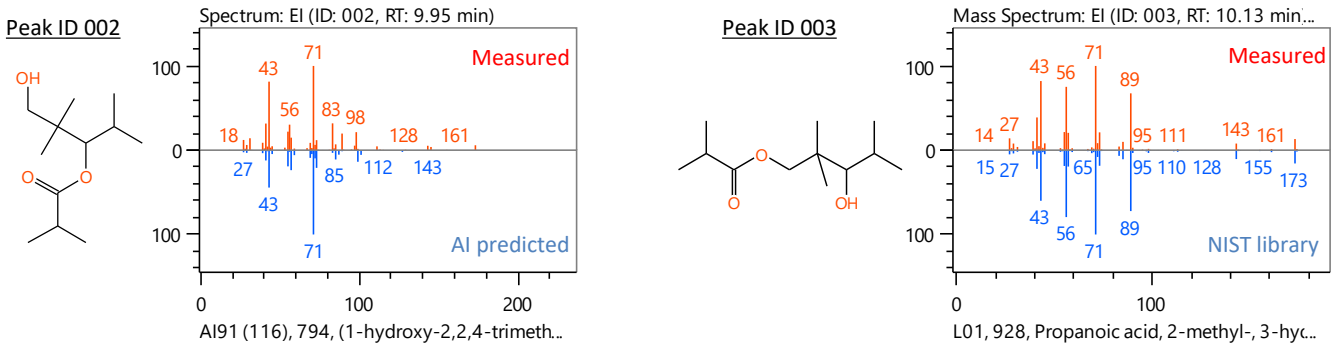

Figure 3 Structure analysis results of peak ID 002 and 003

Conclusion

Using JMS-T2000GC and msFineAnalysis AI, it was possible to obtain the structural formula of TMPMB, which is not registered in NIST library. Additives used in various products are sometimes replaced with alternative substances for a variety of reasons, including regulation, improved performance, and cost reduction. AI structural analysis is effective when qualitative information cannot be obtained using NIST library.

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