GCxGC data analysis of msFineAnalysis AI Ver. 3 ②Polymer pyrolysis

Product used: Mass Spectrometer (MS)

Introduction

The qualitative analysis software msFineAnalysis AI enables automatic structure analysis of unknown compounds not registered in libraries through EI/SI integrated analysis and AI structure analysis. Ver. 3 newly supports comprehensive 2D GC (GCxGC) data analysis. MSTips509 introduced the usefulness of EI/FI integrated analysis using diesel fuel analysis. This MSTips introduces the usefulness of AI structure analysis using polymer pyrolysis analysis. Figure 1 shows a schematic diagram of pyrolysis (Py)-GCxGC-MS. In polymer pyrolysis analysis, some detected compounds not only have unknown mass spectra but also lack known structural formulas. In msFineAnalysis AI system, structural formulas of oligomers generated from the pyrolysis of 49 homopolymers and 18 copolymers are created *in-silico*, and their mass spectra are predicted by AI, enabling qualitative analysis.

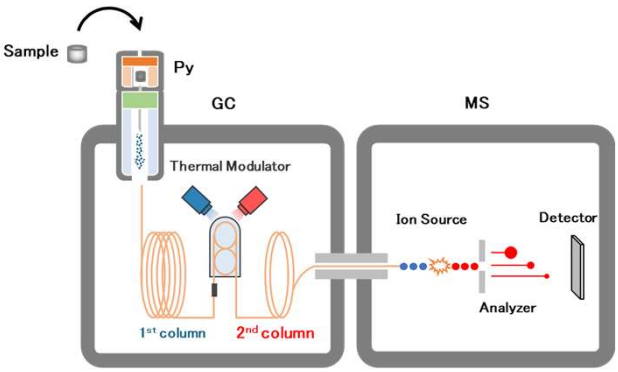

Figure 1 Schematic diagram of Py-GCxGC-MS

Experiment

A commercial styrene-butadiene rubber (SBR) product was used as the sample, and 0.2 mg was weighed. The pyrolysis analysis was performed using a single-shot mode at a furnace temperature of 600C of EGA/PY-3030D (Frontier Laboratories). Detailed analytical conditions are shown in Table 1.

Table 1 Analytical conditions

Pyrolyzer : EGA/PY-3030D (Frontier Laboratories)	
Mode	Single shot
Furnace temperature	600ºC
Gas Chromatograph : 8890A GC (Agilent Technologies)	
Inlet temperature	300ºC
1st column	BPX5 (TRAJAN) 30m, 0.25mm, 0.25µm
2nd column	Rxi-17Sil MS(Restek) 3.4m, 0.15mm, 0.15µm
Oven temperature	40ºC(2min)-5ºC/min -320ºC(30min)
Split ratio	100:1
Carrier gas	He, 2mL/min
GCxGC Modulator : INSIGHT-Thermal modulator (SepSolve Analytical)	
Modulation period	8 sec
Modulation loop length	77cm in 2nd column

Mass Spectrometer : JMS-T2000GC (JEOL)	
Ion Source	EI/FI combination ion source
Ionization	EI : 70eV
	FI : FI emitter, Flashing 12mA 3msec
IS temperature	EI : 250ºC / FI : No heating
GC-ITF temperature	250ºC
Mass range	*m/z* 30-800
Recording interval	EI : 0.02sec(50Hz) / FI : 0.04sec(25Hz)
Drift compensation	EI : PFTBA *m/z* 263.987, reservoir at end time
	FI : PDMS *m/z* 281.051, reservoir every 20min

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Results

Figure 2 shows a screenshot of the analysis result of msFineAnalysis AI.

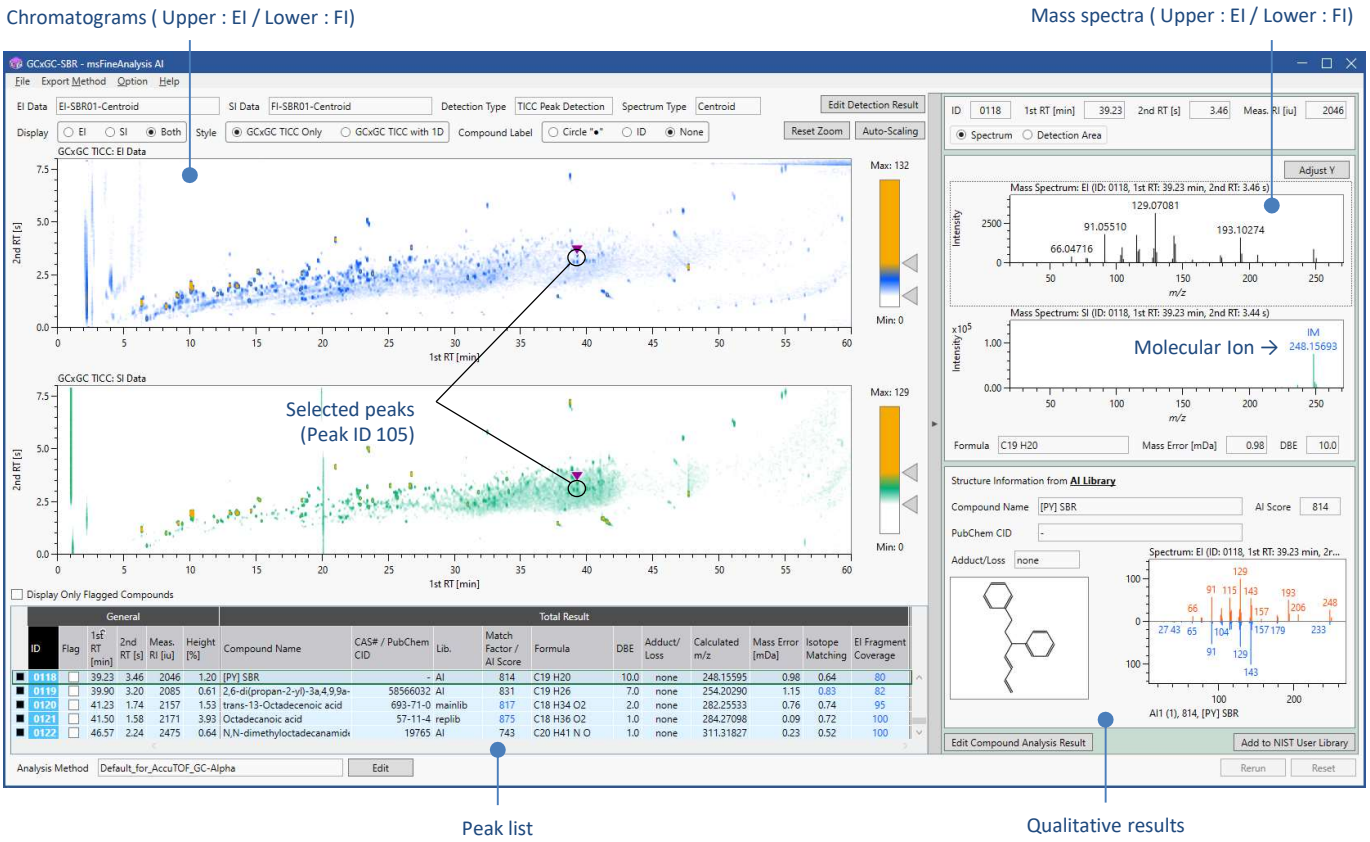

Figure 2 Screen shot of msFineAnalysis AI

Figure 3 shows a screenshot of the AI structure analysis result for peak ID118. Although this compound was not registered in the NIST library, the AI structure analysis suggested a styrene-styrene-butadiene (SSB) hybrid trimer as the top candidate structure.

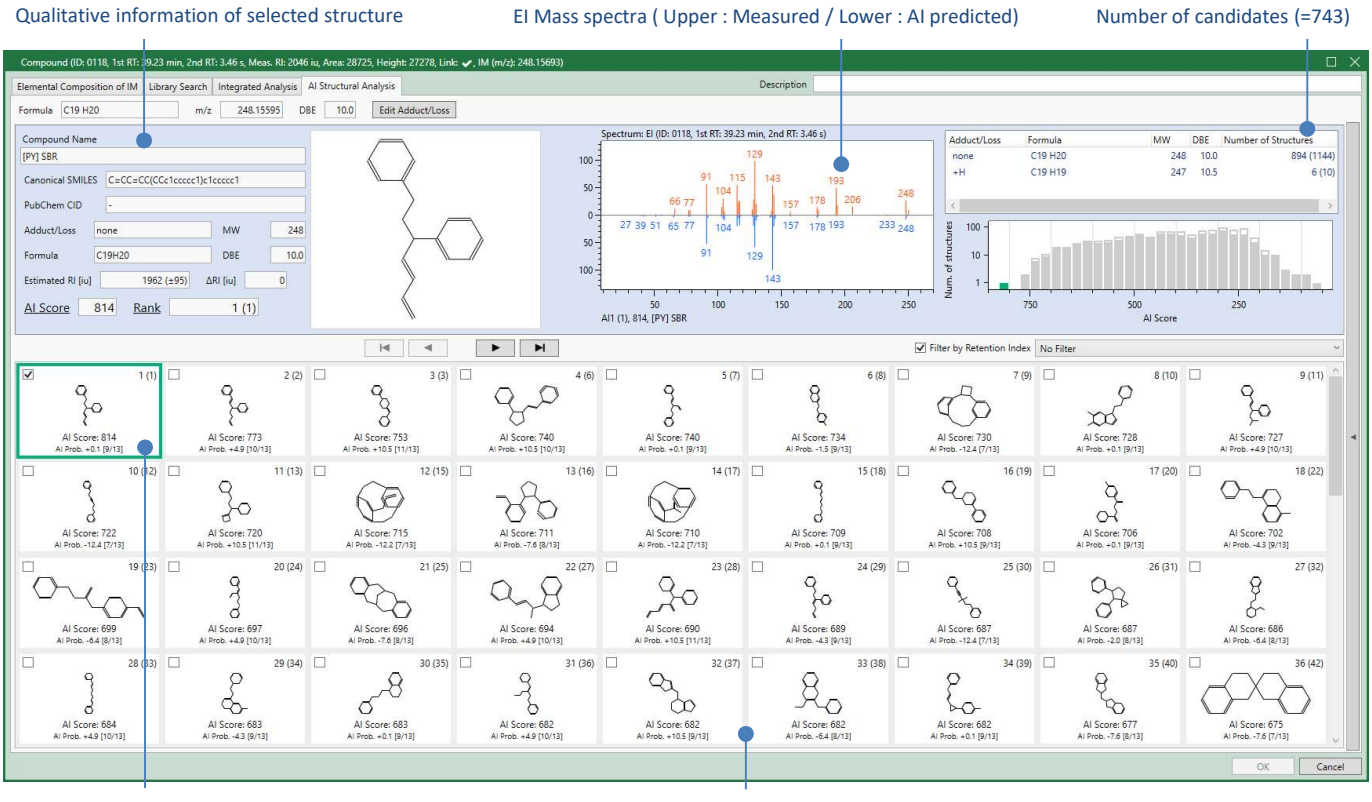

Figure 3 Screenshot of AI structure analysis result

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Figure 4 compares a 1D chromatogram obtained by single GC-MS with a 2D chromatogram obtained by GCxGC-MS. In the 2D chromatogram, styrene-butadiene (SB) hybrid oligomers, which are pyrolysates of SBR, and additives were successfully separated. Additionally, it was observed that SB hybrid oligomers shifted upward along the vertically as the degree of styrene polymerization increased.

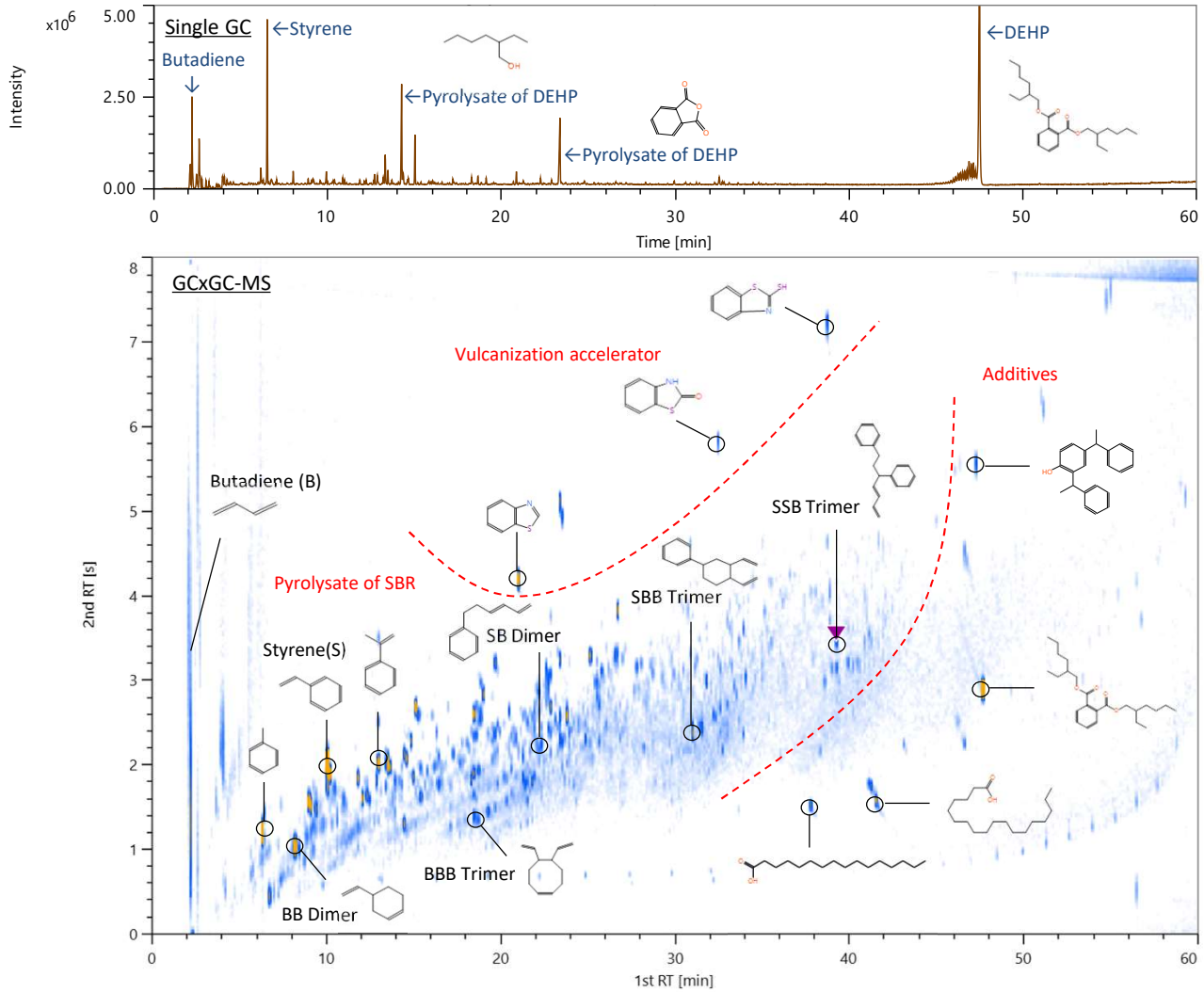

Figure 4 Chromatograms of SBR (Upper : Single GC-MS / Lower : GCxGC-MS)

Conclusion

With the new support for GCxGC data analysis in msFineAnalysis AI Ver.3, it is now possible to automatically obtain structural formulas for unknown compounds detected in 2D chromatograms through AI structure analysis.

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