

# Application for Forensic Analysis: Discrimination of Fibers using Trace Organic Additive and Pyrolyzate Marker

Chikako Takei, Kenichi Yoshizawa; BioChromato, Inc.

## Introduction

Forensic analysis of evidence collected at a crime scene is required for criminal investigations.

Direct Analysis in Real Time Mass Spectrometry (DART®-MS) is an ambient ionization method reported by Robert B. Cody et al. in 2005 [1]. It is excellent in versatility and speed, as organic samples are easily ionized at atmospheric pressure directly in front of a mass spectrometer. However, some target compounds are challenging to identify using DART® as an ion source such as polymers, cloths, fibers, or plastics. Therefore, we developed a thermal desorption and pyrolysis (TDP) device coupled with DART®-MS, capable of directly heating the sample from room temperature to 600 °C in a controllable manner. TDP/DART®-MS can be utilized to identify additives in the lower thermal desorption region and polymer matrices in the higher pyrolysis region from polymer material products. In this presentation, it is shown that TDP/DART®-MS can be used for both identification and comparison of polymer material products.

[1] R. B. Cody, J. A. Laramée & H. D. Durst, Anal. Chem., 77, 2297-2302 (2005)

## Materials and Methods

### Samples

6 types of white polyester sewing threads (commercial products)

### Analytical methods: TDP/DART®-MS (Fig. 1)

Sample (ca. 0.2 mg) were used for measurement.

Mass Spec.: Compact (Bruker)  
 Ion Source: DART®-SVP (IonSense)  
 Ionization gas: Helium  
 Helium gas temperature: 400°C  
 TDP device: ionRocket (BioChromato)  
 Temperature program : RT → 600°C(100°C/min)

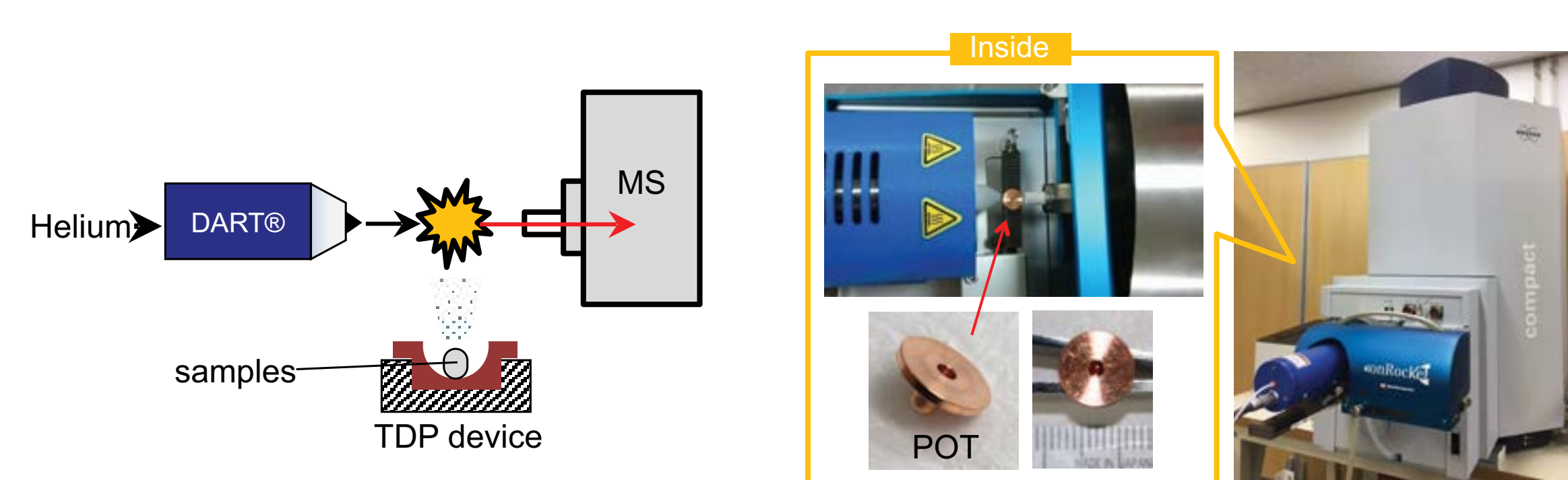


Fig. 1 TDP/DART®-MS System.

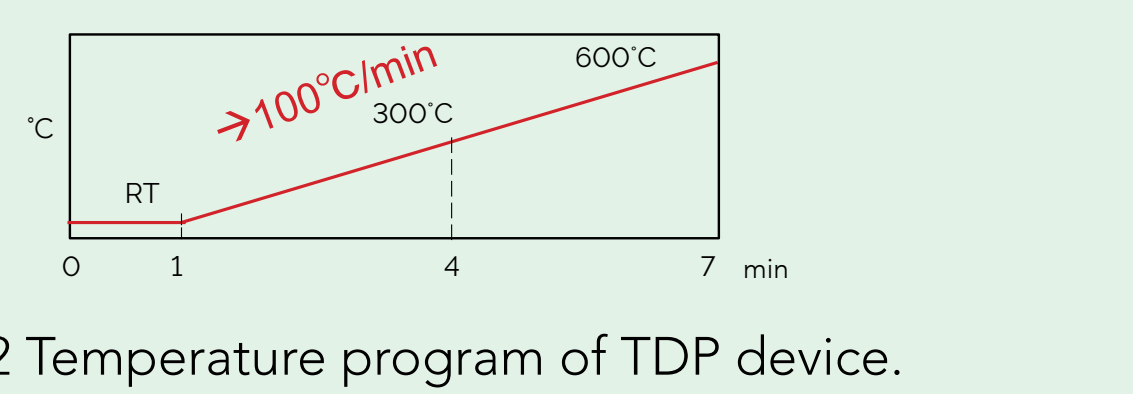
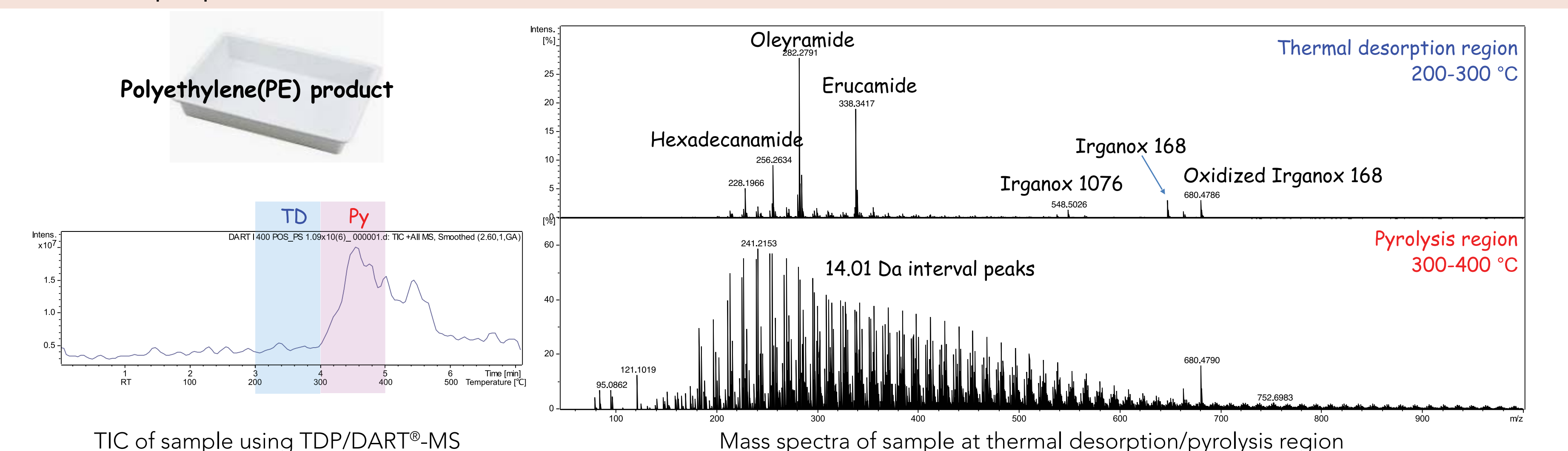


Fig. 2 Temperature program of TDP device.

### Introduction for TDP/DART®-MS data

This method enables acquisition of both additives in the thermal desorption region and polymer pyrolyzates in the pyrolysis region, without sample pretreatment.



This analytical method is a powerful tool for rapid & easy identification of compounds.

## Results and Discussions

### Reproducibility of TDP/DART®-MS

Overlaying of TIC and EIC shows good reproducibility.

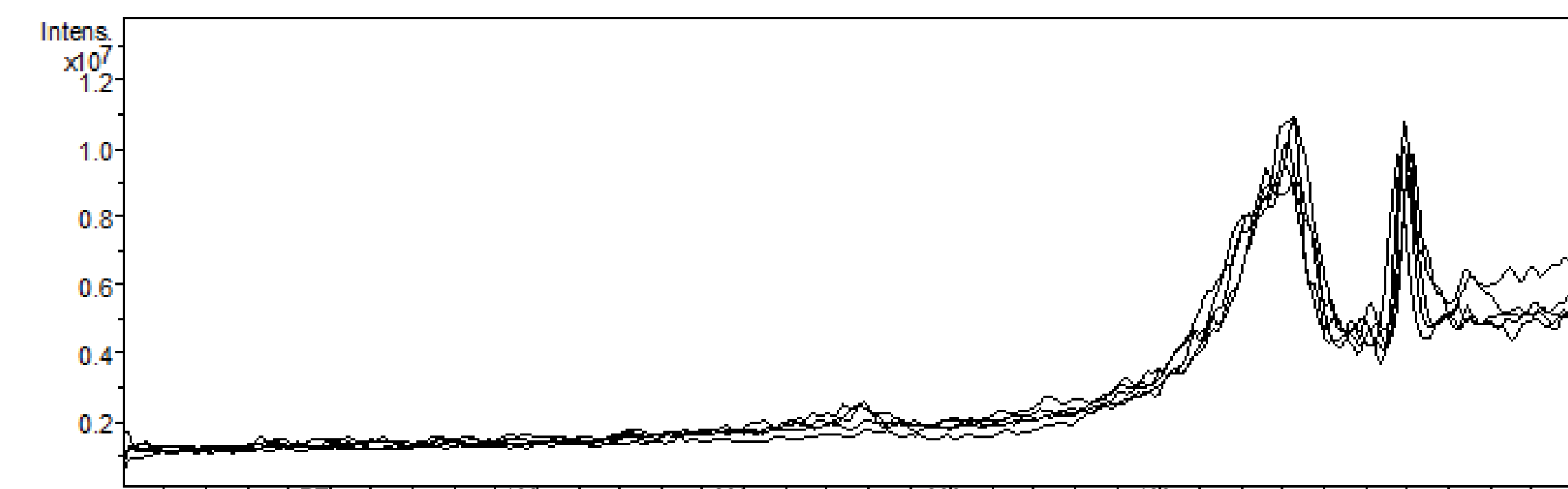


Fig. 2 Overlaying of TIC using TDP/DART®-MS

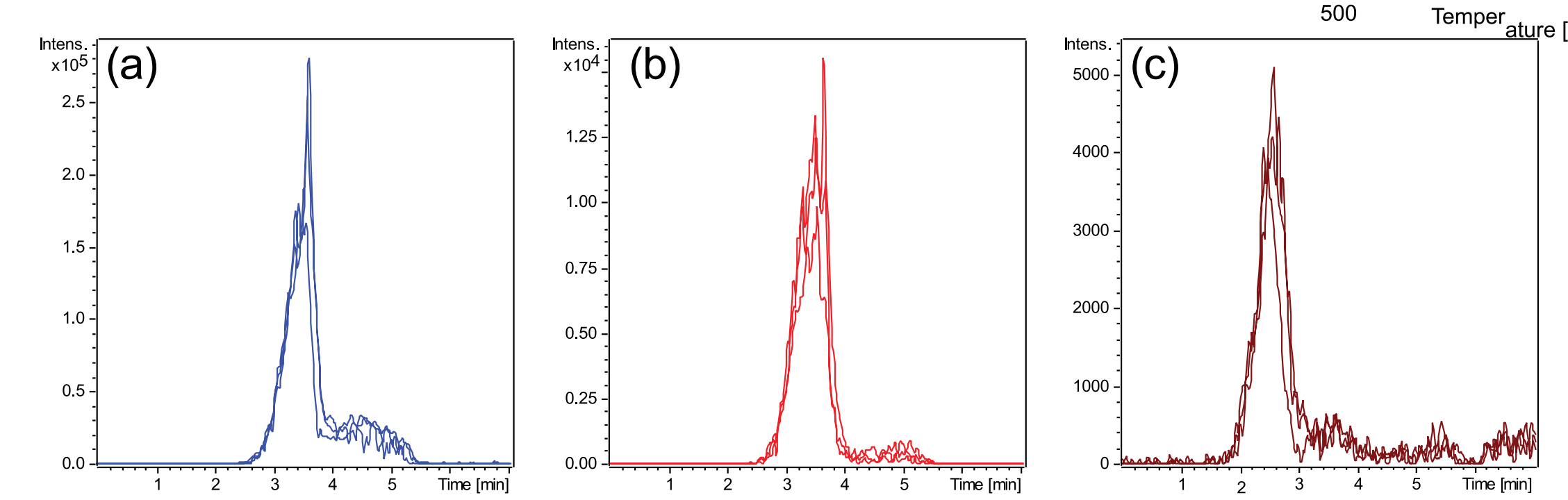
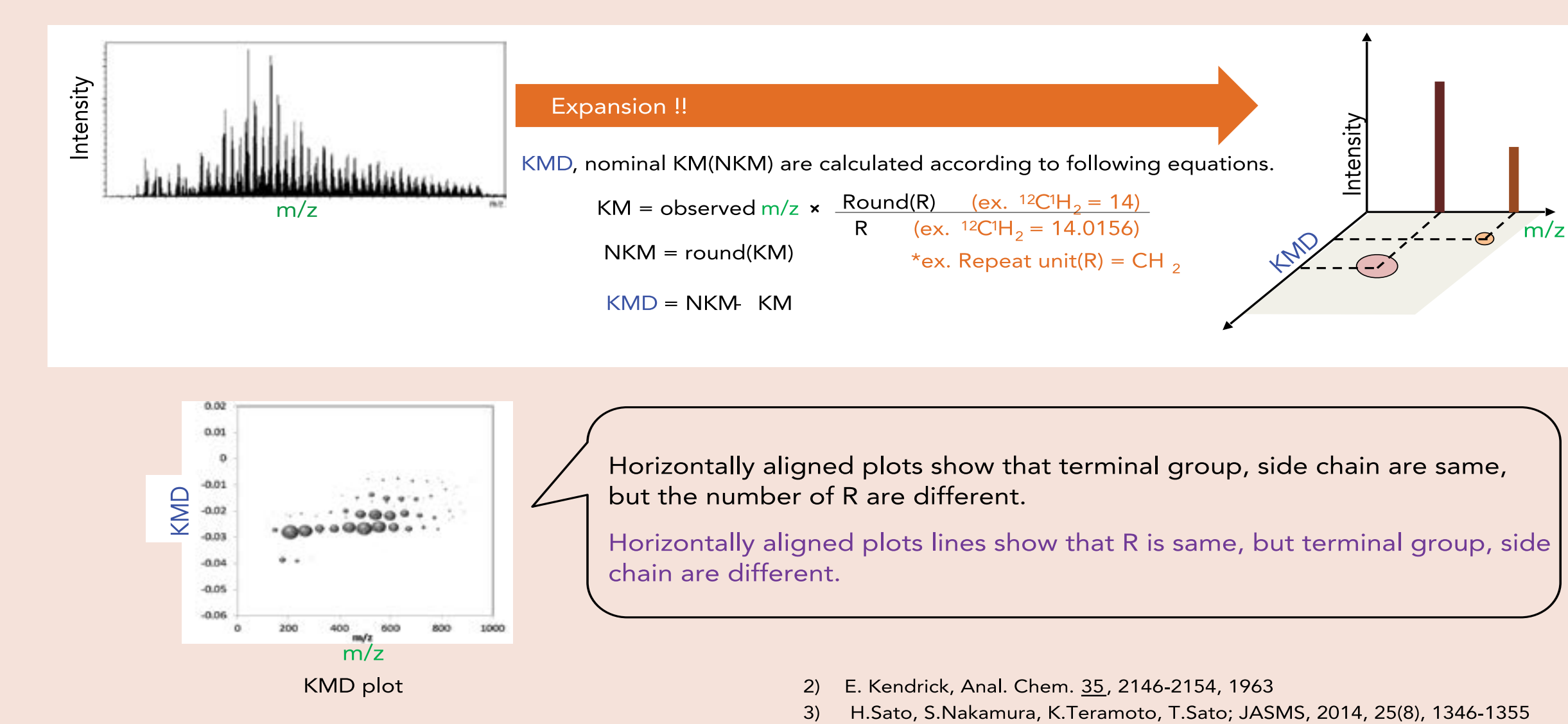


Fig. 3 Overlaying of EIC using TDP/DART®-MS;  
 (a) m/z 291.11; phosphate ester type additive, (b) m/z 600.52; fatty acid amides (FAAs),  
 (c) m/z 350.32; polyethylene glycol ethers of tridecyl alcohol.

Table 1. Reproducibility for EIC peak area by TDP/DART®-MS

	Peak area value (n=4)				Average	Standard Deviation	Coefficient of variation
m/z 291.11 ±0.001	9045346	8662186	9411450	8470357	8897334.8	417862.3	4.7%
m/z 600.52 ±0.001	438070	490901	482518	474295	471446.0	23260.6	4.9%
m/z 350.32 ±0.001	151063	156313	165768	153401	156636.3	6455.5	4.1%

### Kendrick mass defect (KMD) plot<sup>2,3</sup>



## Conclusion

By using TDP/DART®-MS, additives contained in sewing threads and polyester pyrolyzates were detected in the thermal desorption region and pyrolysis region, respectively. Moreover, all the samples were distinguished by using additives and pyrolyzates as markers. Thus, this analysis method is useful for discrimination of not only sewing threads but also plastic products.

### Results of Discrimination

Characteristic mass peaks of additives were observed in each sample, in the thermal desorption region.

Polyester types were identified by analyzing pyrolysis mass spectra.

A KMD plot was useful for finding the difference among samples.

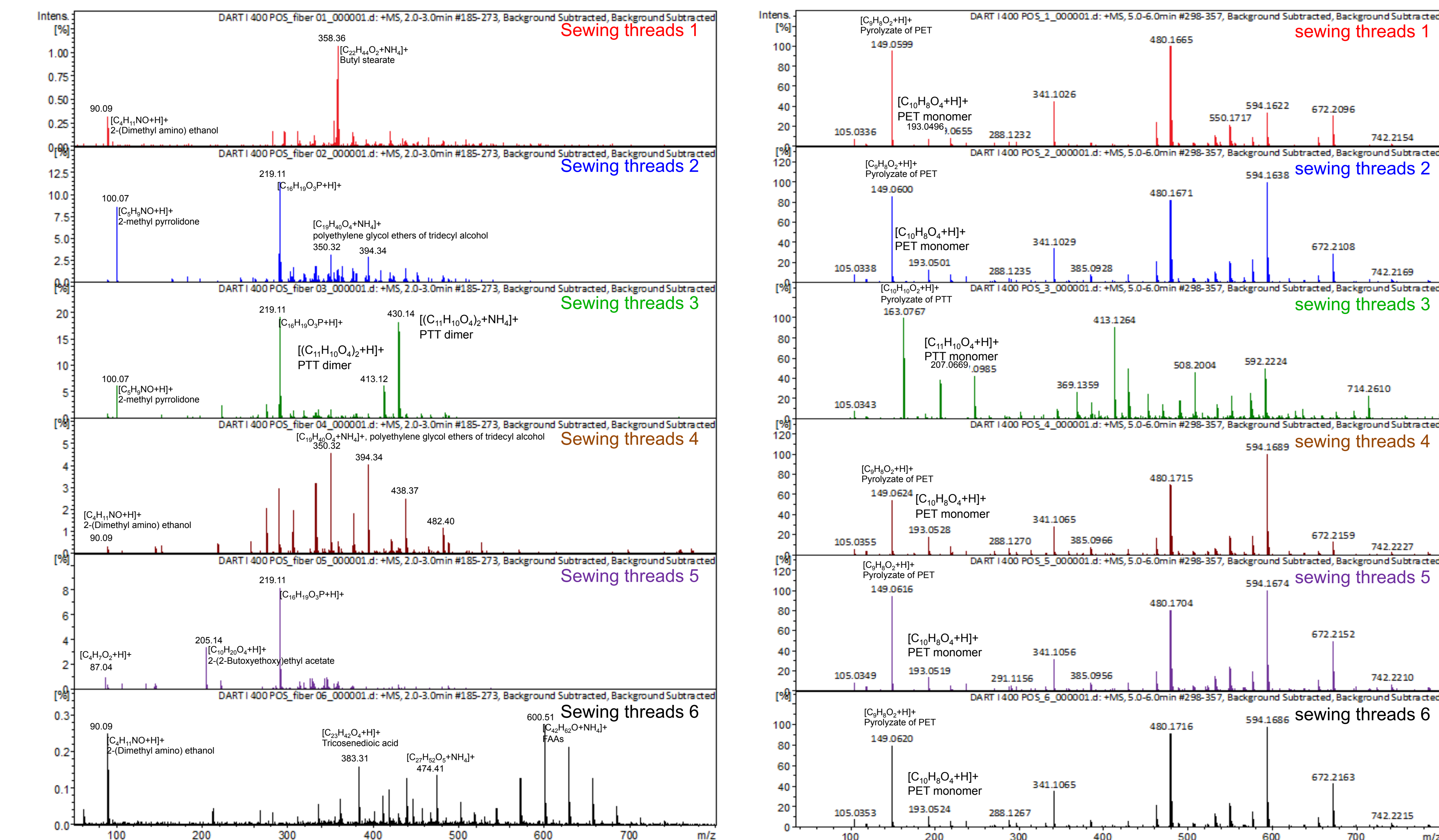


Fig. 4 Mass spectra of at thermal desorption region using TDP/DART®-MS

Fig. 5 Mass spectra of at pyrolysis region using TDP/DART®-MS

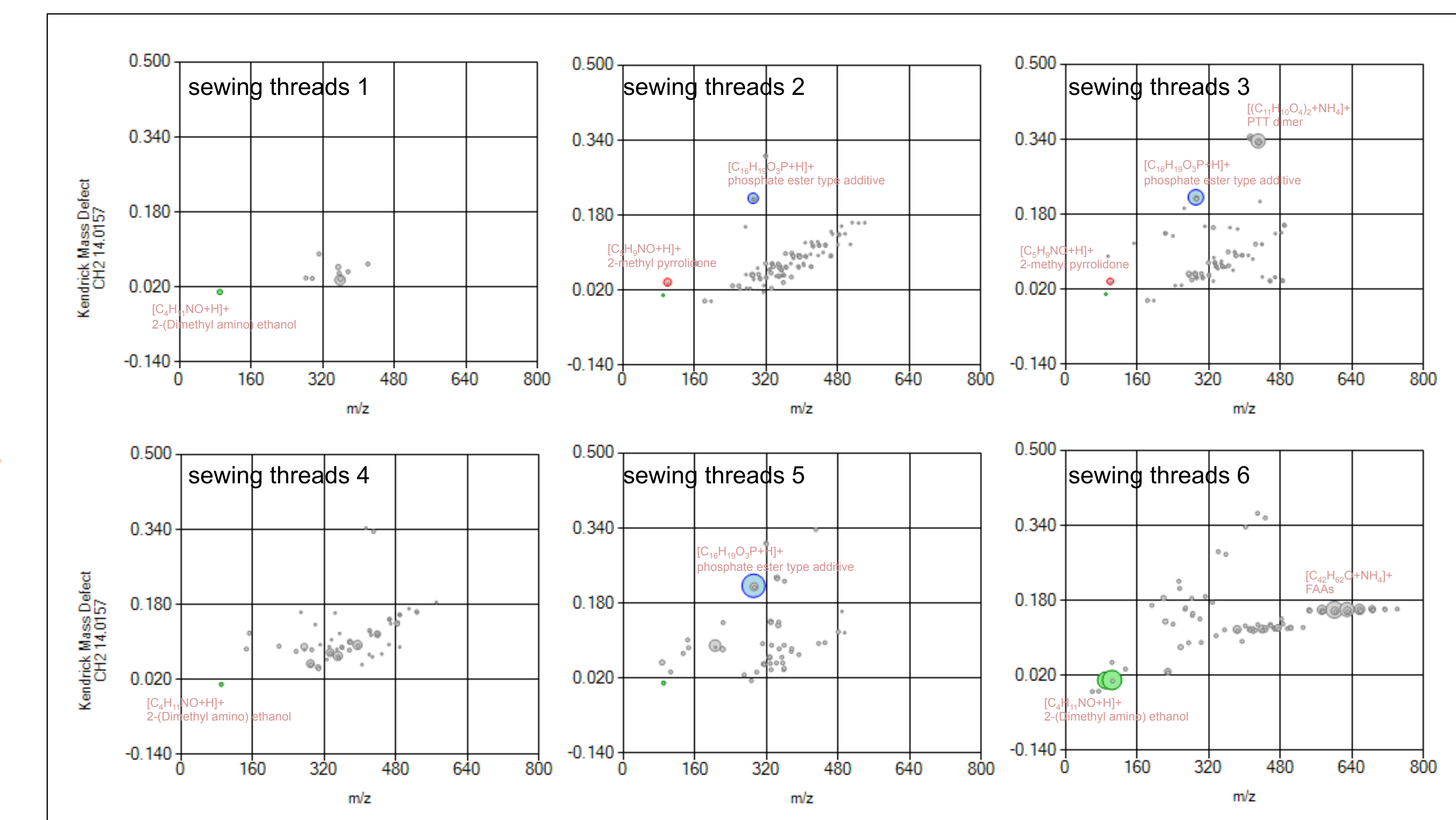


Fig. 6 KMD plots converted from mass spectra at thermal desorption region, (base unit: CH<sub>2</sub>)