

Deconvolution of Plastic Mixtures using a Polymer Subtraction Function in Py-GC-MS Data Analysis Software

Application Note

General

Abstract

This application note demonstrates a polymer subtraction capability in Py-GC-MS-data analysis software.

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Introduction

A pyrogram of a pure polymer can be complex, and interpretation requires a polymer mass spectrum database as well as analyst knowledge. As a result, a mixture of polymers can be even more difficult to interpret. A recent application note described novel mass spectral processing software with a Compound Subtraction Feature, which was utilized to deconvolute a mixture of polypropylene and polyethylene¹. This application note took a similar approach to analyze a different polymer mixture.

Results and Discussion

It is straightforward to perform a search in MSChrom from the Py-GC-MS database on a pure polymer sample, however many real-world samples involve more than one polymer, so a simple mass spectral search may provide limitations. Here, a novel Compound Subtraction function, part of CDS Mnova Plugin, built into MSChrom software, was used to subtract one polymer from a two-polymer mixture. The mixture was first pyrolyzed at 700°C using Py-GC-MS and then the data was brought over to MSChrom. The mixture's peaks were combined into a single spectrum using The Crosshair Select Tool (Figure 1) and searched against the pyrolysis database.

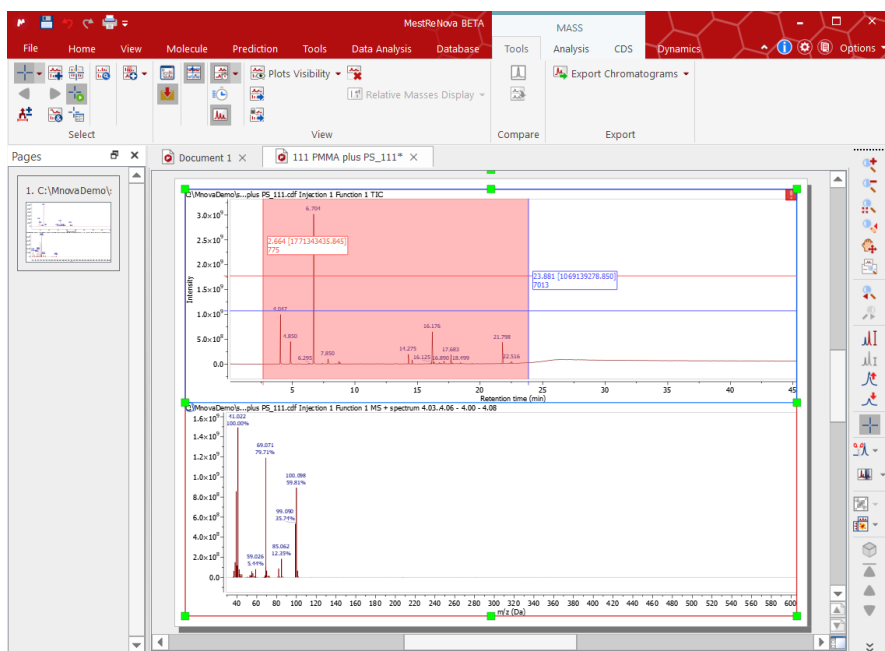


Figure 1. Combining Peak Spectra for a database search.

The database search's top record was polystyrene (Figure 2). Polystyrene data was added to MSChrom and the two chromatograms were stacked so they could be compared; a peak in the mixture at 4 minutes which was not in polystyrene confirms the presence of a second material (Figure 3).

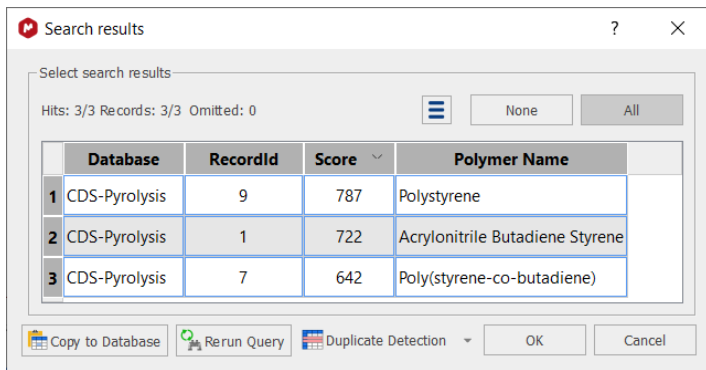


Figure 2. Mixture Search Results

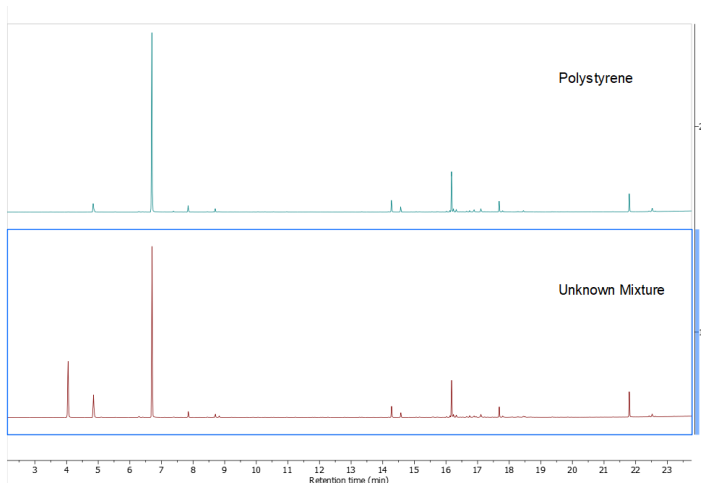


Figure 3. Polystyrene (top) vs. Unknown Mixture (bottom).

To subtract the polystyrene polymer from the mixture, the Compound Subtraction Tool, which allows for peak alignment and subtraction was selected under the CDS ribbon (Figure 4).

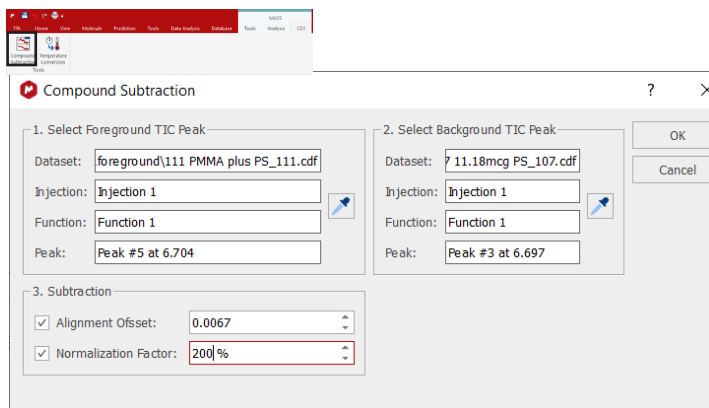


Figure 4. Compound Subtraction Interface.

Using the interface, polystyrene's largest peak, styrene, at 6.67 minutes, was aligned on the x-axis (retention time) to the same peak in the mixture by graphically selecting them in each plot; a normalization factor was calculated to allow the background pyrogram to match the intensity of the mixture and selecting "OK" performed the subtraction. Figure 5 shows that the aligned peak as well as others associated with polystyrene have been minimized and the peak at 4 minutes was the most abundant in the

chromatogram after subtraction. When the compound subtracted pyrogram was searched against the pyrolysis database a new top match of polymethyl methacrylate replaces the polystyrene match (Figure 6).

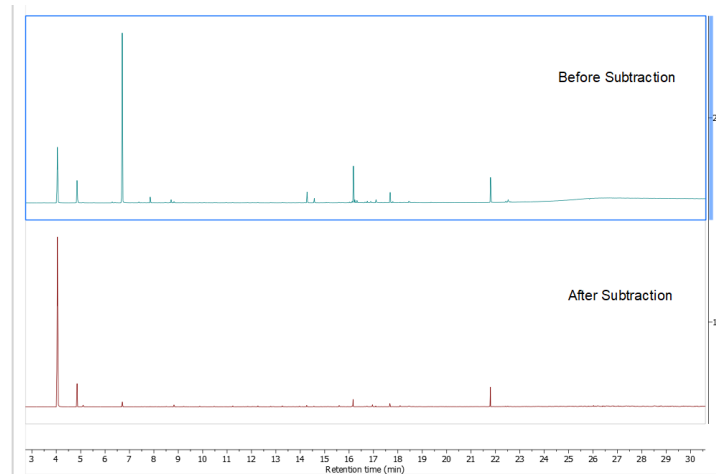


Figure 5. Mixture before (top) and after (bottom) Compound Subtraction.

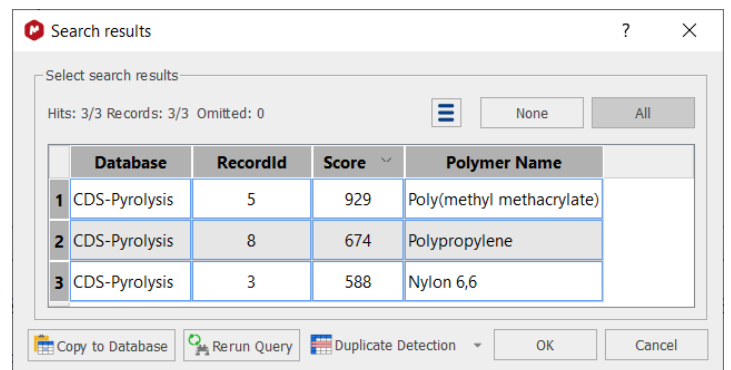


Figure 6. New Search on Compound Subtracted Data reveals new top Record (polymethyl methacrylate).

The mixture's pyrogram now more closely resembles a polymethyl methacrylate (Figure 7), indicating that the unknown is a mixture of polystyrene and polymethyl methacrylate.

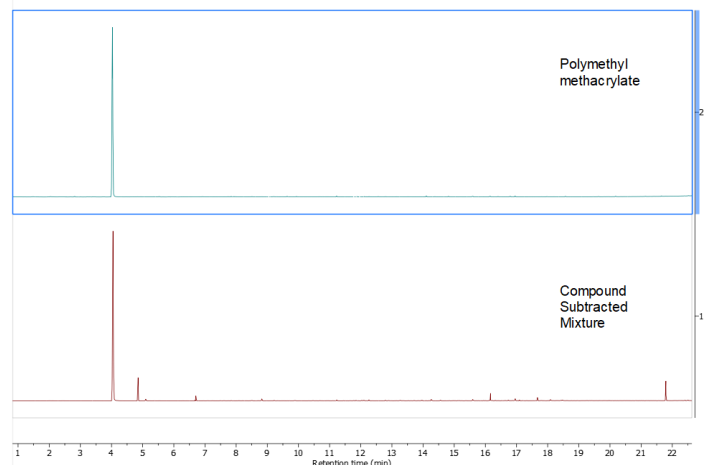
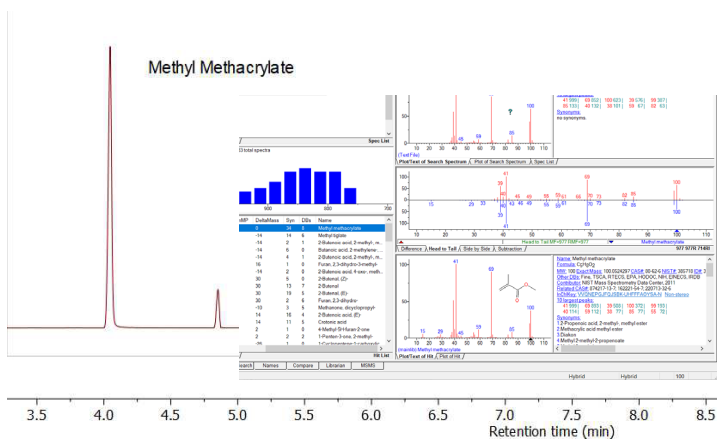


Figure 7. Polymethyl methacrylate (top) and Mixture after Compound Subtraction (bottom).

Additionally, MSChrom can access the NIST search engine and database to identify individual compounds, if installed. Figure 8 shows methyl methacrylate, the monomer of polymethyl methacrylate, identified using the NIST search engine which was accessed through MSChrom (Figure 8).



Conclusion

There are difficulties in interpreting Py-GC-MS data; mass spectrum databases and analyst expertise are some of the methods used. Here, a mixture consisting of polystyrene and polymethyl methacrylate was broken down using a novel compound subtraction tool in MSChrom in conjunction with a polymer pyrolysis database.

References

1. Sam, K. "Enhancing Characterization of Mixed Polymers with a Mass Spectral Processing Software for Py-GC-MS", CDS Application Note #281.