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Discrimination Between Commercial Lubricant Oils Using Mass Spectrometry and Multivariate Analysis within UNIFI Software

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This is an Application Brief and does not contain a detailed

Experimental section.

Abstract

In this technical note we outline a simple and efficient workflow that uses high resolution mass spectrometry and statistical analysis of the acquired data to understand the differences between two car lubricant oils at a molecular level. This approach could be particularly useful in comparing two similar products, identifying the differences between poorly performing and correctly performing oils, or deformulating competitor's products.

Benefits

- Demonstrate the power of high resolution accurate mass data acquisition for the analysis of complex samples, such as lubricant oil formulations.
- The use of multivariate statistical tools within UNIFI Software in a quick and simple automated workflow to understand the differences between samples

Introduction

Lubricant oils are used in a vast array of industrial applications, from domestic car engines, to oil well drilling rigs, to specialist metal-working machinery; in fact, lubricant oils may be found in any situation where surfaces might contact one another and friction become a problem.[1,2] Due to their wide range of uses, many different formulations of lubricant oils are manufactured.

Typical lubricant oils are comprised of a base oil, which can be either a mineral oil or a synthetic oil, and specialist additives. Mineral oils are refined from naturally occurring crude oil whereas synthetic oils are manufactured from long-chain hydrocarbon-based molecules known as polyolefins. Additive packages are then combined with the base oil to provide specific performance characteristics and to offer protective properties to both the oil and the mechanical system.[2,3]

A variety of approaches can be used to understand the quality and condition of a lubricant oil.[4-7] In this technical note we outline a simple and efficient workflow that uses high resolution mass spectrometry and statistical analysis of the acquired data to understand the differences between two car lubricant oils at a molecular level. This approach could be particularly useful in comparing two similar products, identifying the differences between poorly performing and correctly performing oils, or deformulating competitors' products.

Results and Discussion

Two generic lubricant oils, targeted to different makes of cars, were prepared at a concentration of 0.5 mg/mL. The samples were infused into a Waters SYNAPT G2-S*i* HDMS System using electrospray ionization in positive ion mode. UNIFI software was used for data processing and EZInfo for MVA statistical analysis.

High resolution data for two lubricant oils and a solvent blank were acquired in triplicate. The nine data files were processed in UNIFI using an accurate mass screening analysis method which resulted in a collection of candidate components for each sample. Detected components, considered to be the same within an acceptable *m/z* tolerance, were collected together across the samples into markers. The markers were transferred from UNIFI directly into EZInfo and analyzed using Principal Component Analysis (PCA). The resulting scores plot shown in Figure 1, indicates excellent grouping between the replicates for each sample type and highlights that there are significant differences between the lubricant oils.

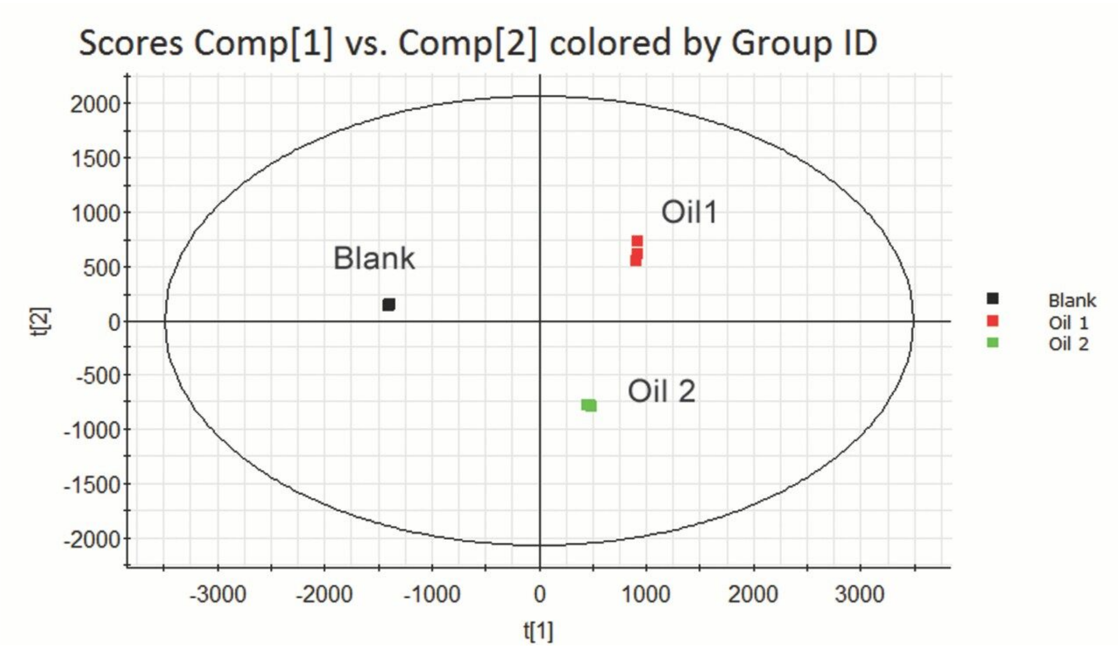

Figure 1. PCA scores plot showing clear grouping of each lubricant oil and the blank.

The markers responsible for the differences between sample types can be determined from the associated loadings plot. Figure 1 shows that the samples for each lubricant oil and the blank are grouped in specific regions of the scores plot. Markers responsible for the differences between the samples are grouped in similar regions of the associated loadings plot shown in Figure 2. The markers elevated in each lubricant oil lie within the trajectories highlighted in Figure 2.

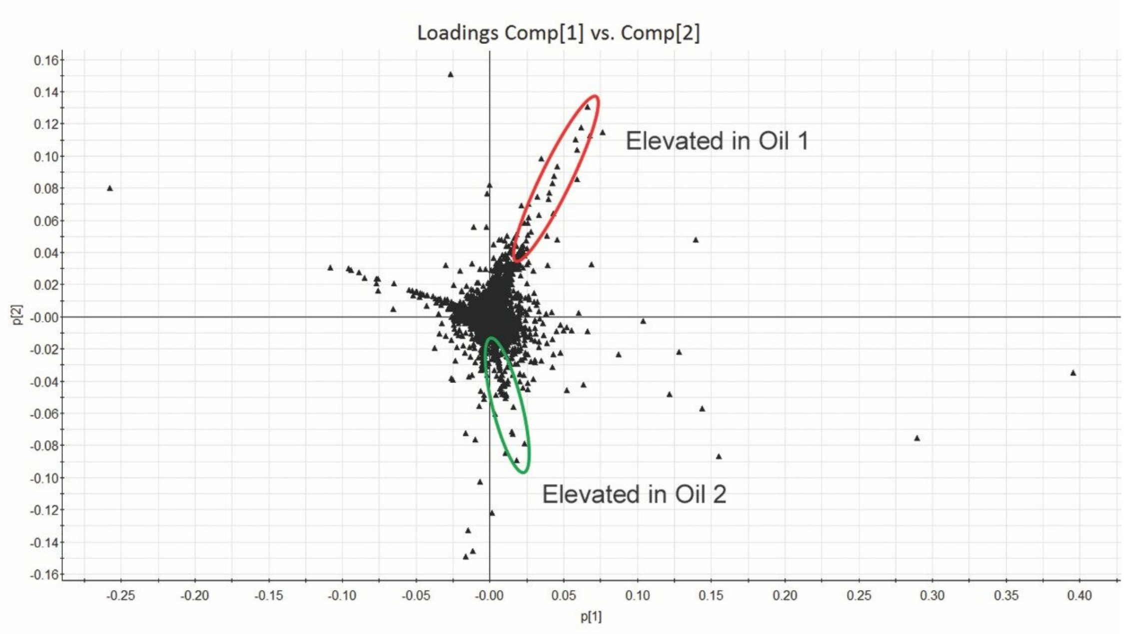

Figure 2. PCA loadings plot with the markers elevated in lubricant oil 1 (red ellipse) and lubricant oil 2 (green ellipse).

The trends of five markers, from each trajectory highlighted in Figure 2, are plotted in Figure 3 across all samples and clearly show elevated responses for one of the lubricant oils.

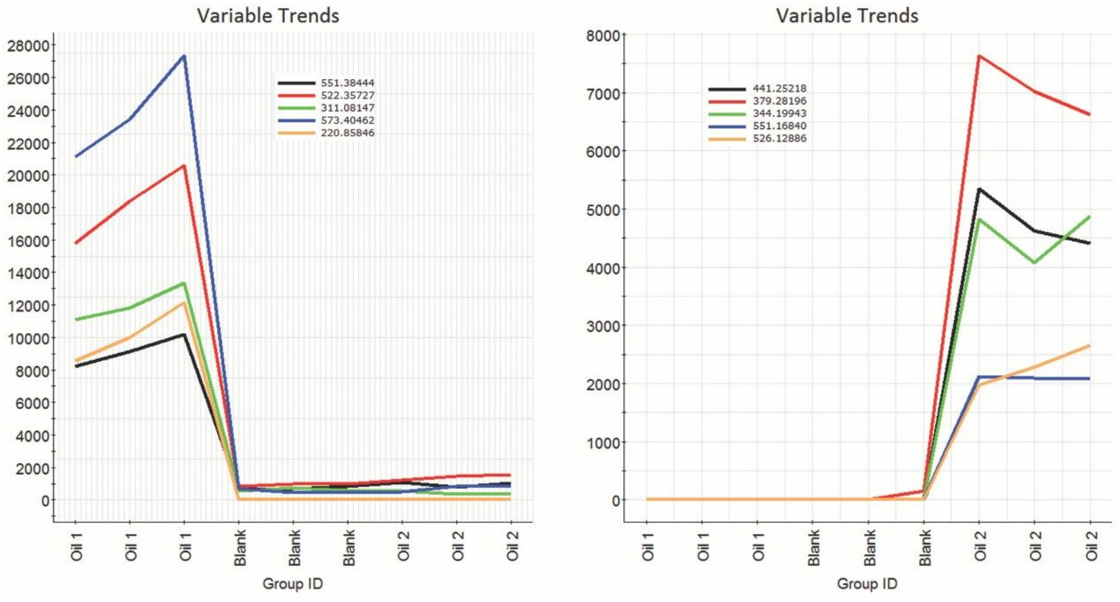

Figure 3A. Shows examples of markers elevated in oil 1, compared to the blank and oil 2; 3B shows examples of markers elevated in oil 2, compared to the blank and oil 1.

Table 1 shows the *m/z* values of the five selected markers that have an elevated response in each of the lubricant oils. Even though the compounds represented by these *m/z* values have not been identified, it is still possible to create library entries for them in UNIFI and target them when processing data within UNIFI.

The lubricant oil data were subsequently screened against the new library. The relevant markers were detected in the appropriate samples, e.g. *m/z* 522.3572 was elevated in lubricant oil 1 and *m/z* 344.1994 was only detected in lubricant oil 2. Summary plots for these two detected targets are shown in Figure 4. Similar summary plots were produced for the other eight targets.

Marker for oil 1	Marker for oil 2
551.3844	441.2521
522.3572	379.2819
311.0814	344.1994
573.4046	551.1684
220.8584	526.1288

Table 1. m/z values of markers with elevated responses in one of the lubricant oils.

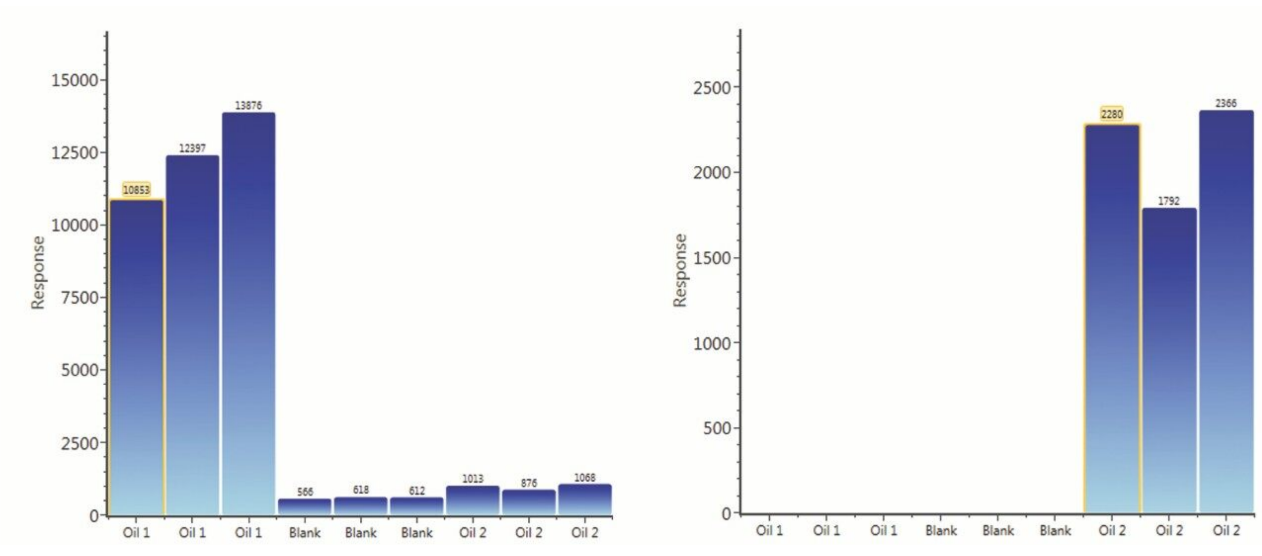

Figure 4. UNIFI Component Summary plots showing the markers with A. m/z 522.3572, and B. m/z 344.1994, across all samples.

Conclusion

It has been demonstrated that mass spectrometry combined with appropriate informatics can be used to differentiate between two commercially available lubricant oils. A straightforward workflow has been presented and is illustrated in Figure 5.

Figure 5. Workflow employed to discover differences between two lubricant oils.

This workflow could be used for a variety of industrial applications, e.g. to discover changes to a lubricant oil as it is stressed. An additional step to the workflow would be to further characterize the components that are found to differentiate between lubricant oils, thus providing specific information on their different compositions.

References

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