[TECHNOLOGY BRIEF]

HDMS Compare Software for Complex Materials Comparisons

GOAL

To demonstrate the utility of novel HDMS Compare software for the comparison of complex asphaltene samples analysed using Waters® Atmospheric Solids Analysis Probe (ASAP) with SYNAPT® G2 HDMS™, which incorporates ion mobility functionality.

BACKGROUND

Many industries routinely handle complex samples on a daily basis. Examples of such analytes include crude oil, bio-oil, crude oil fractions and derivatives, advanced polymer blends, and complex chemical formulations.

Typically, numerous analytical tools are used to investigate and characterize these samples – including various mass spectrometric techniques. The data acquired reflect the complexity of the materials being analyzed and contain myriad components. Consequently, data analysis is a significant challenge, requiring powerful and intuitive tools that are functional and easy to use on a routine basis.

Frequently, it is necessary to make comparisons between complex samples; for example when a particular compound fails to perform correctly, or the same sample has been treated or processed in different ways. In these cases, a visual comparison of data from the samples is extremely difficult, and identifying key differences is particularly problematic.

A software tool that facilitates the identification of important analyte differences, by carrying out automated data comparisons, offers a valuable approach to help overcome this bottleneck in data analysis workflows.

HDMS Compare software is a powerful tool for rapid and simple comparison of complex samples.

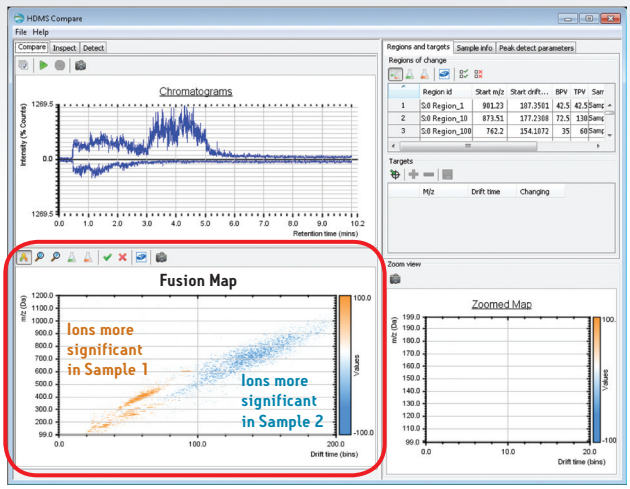

Figure 1a. Comparison between the full data acquisitions for two different asphaltene samples.

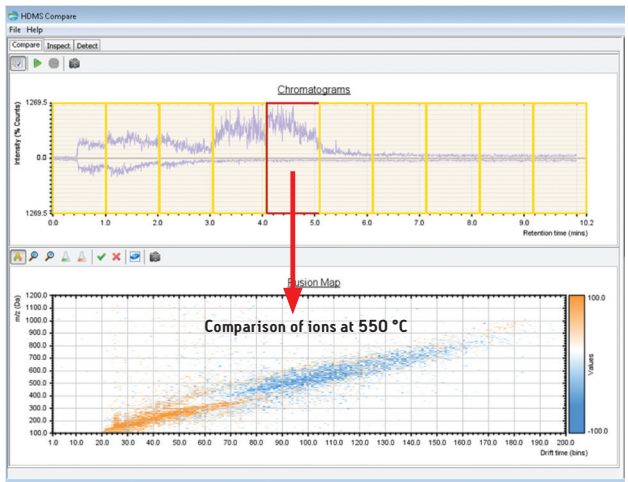

Figure 1b. Comparison between the data "slices" at 550 °C (4 to 5 minutes).

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THE SOLUTION

The analysis of different asphaltene samples was accomplished using a SYNAPT G2 HDMS instrument, with ASAP for sampling and ionization.

The asphaltenes were made into a thick slurry using toluene. The ASAP facilitated the use of a simple dip technique for rapid, direct sampling of the asphaltene samples. Ionization of the samples was then achieved via traditional Atmospheric Pressure Chemical Ionization (APCI) mechanisms. A manual, stepwise temperature ramp was implemented over the range 150 °C to 650 °C, with 100° increases after every minute elapsed, and a total acquisition time of 10 minutes.

The ion mobility data were then processed using HDMS Compare software. Figure 1a shows the initial view of data from the comparison of two different asphaltenes. The orange regions in the mobility image (Fusion Map) indicate ions that are more significant in Sample 1, and the blue regions indicate ions that are more significant in Sample 2. The software also offers the ability to apply "slices" to the data set, which then allows specific sections of the data to be viewed in isolation. Figure 1b shows the differences between the two samples, at 4 to 5 minutes, when the samples were at 550 °C.

To help identify ions that are significantly different in each sample, the analyst can zoom in to specific regions of the Fusion Map and custom select regions of interest. Figure 2 shows an example of a custom selected region, which then appears in the Zoomed Map and the list in the top right corner reduces to contain only the ions selected. These ions can also be exported into MassLynx for additional interrogation, if required.

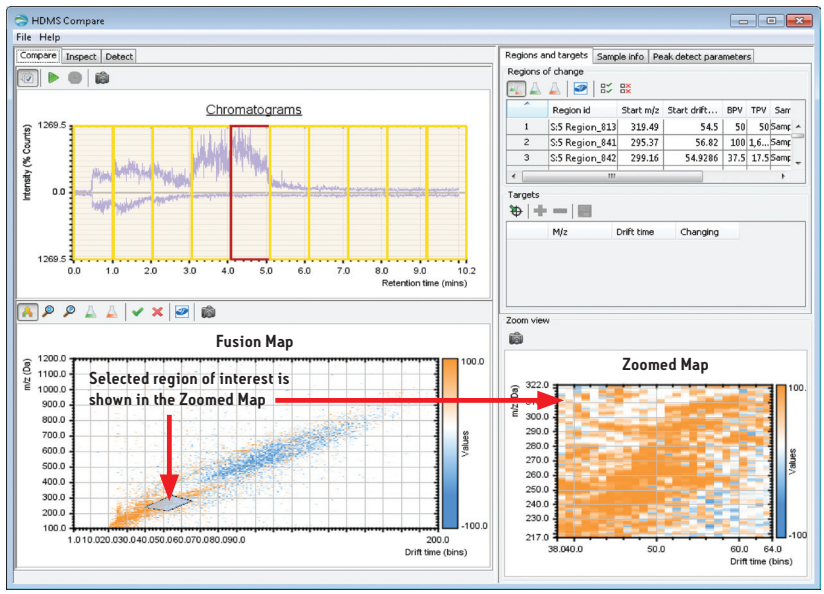

Figure 2. Regions of interest can be selected and zoomed.

SUMMARY

Novel HDMS Compare software was successfully used to make comparisons between mobility data for different asphaltene samples. The samples were analysed using an ASAP-SYNAPT G2 HDMS system, which enabled rapid sampling and data acquisition.

Key areas of significant differences between two samples were clearly visualized and identified with two different, contrasting colours. Regions of interest were easily selected in "slices", or expanded in the Zoomed Map view – this allowed further detailed interrogation of important sample differences.

HDMS Compare software offers analysts, who are frequently required to draw important analytical conclusions based on comparisons between complex samples, a powerful and versatile interactive tool to facilitate their decision making workflow.

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Waters Corporation
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com