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應用手冊

Characterizing Petrochemical Mixtures with Direct Sample Introduction and High Definition Mass Spectrometry

Waters Corporation

Abstract

This application brief provides an in-depth mass spectral analysis of complex samples with direct sample introduction utilizing Atmospheric Solids Analysis Probe (ASAP) and High Definition Mass Spectrometry (HDMS).

Benefits

ASAP-IMS-MS shows the potential to fingerprint crude oil samples, and offers a route to the analysis of involatiles, which cannot be achieved using GC-MS.

Introduction

The chemical characterization of complex mixtures like crude oil remains an extremely challenging problem. In the case of crude oils, the rarefaction of these natural resources results in the use of heavier products, which need to be characterized. Techniques like FTMS or 2D-GC-MS are commonly used, but there are limitations in the MS separation of isomers. In the case of GC, chromatography is limited to low volatility compounds. The

separation of isomers using ion mobility has been explored for some time using experimental instruments, but is now available commercially. Most of the initial applications have been published in the domain of natural polymers, such as proteins. However, other studies have been conducted using ion mobility on experimental instruments in the domain of crude oil[1]. In this technology brief we explore the potential of a commercial instrument, the Waters SYNAPT G2 HDMS, for the characterization of industrial products, including crude oil.

Results and Discussion

Direct sample introduction of a crude oil sample and ionization was performed using the ASAP technique with the SYNAPT G2 HDMS Mass Spectrometer. The conventional Tof-MS spectrum obtained is extremely complex, as shown in Figure 1.

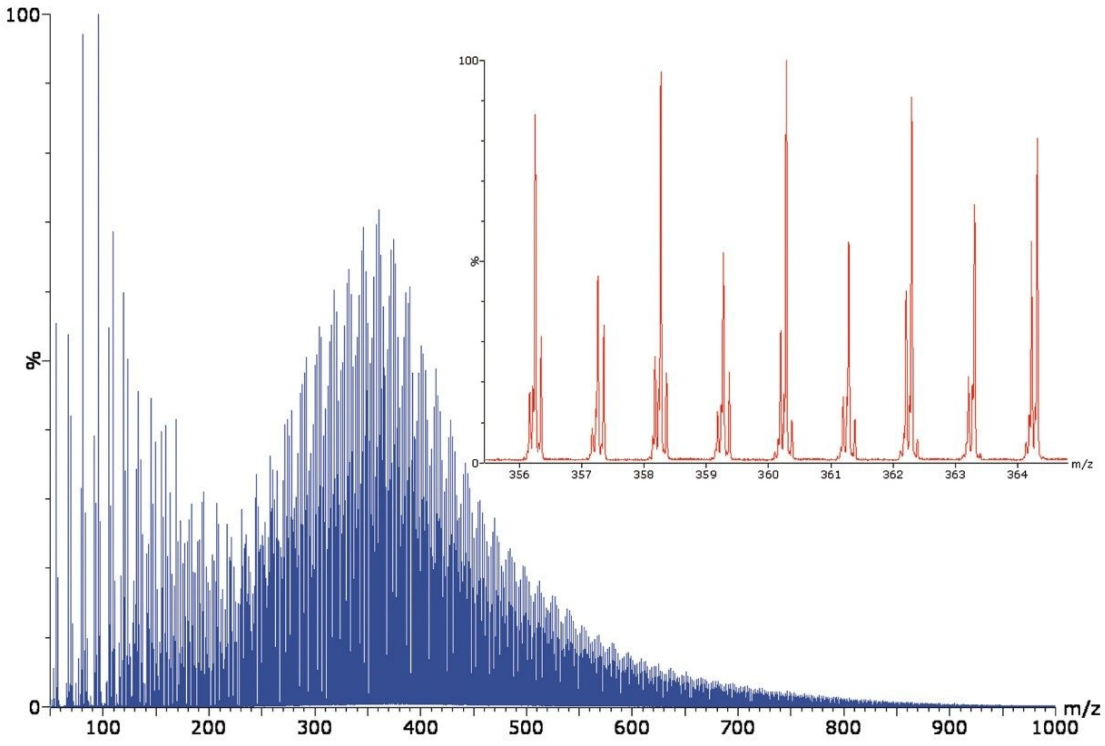

Figure 1. Spectrum for a crude oil sample, with close-up view of a 10 Da window.

When using ion mobility separation, bands separated by 14 Da (CH2) are visualized, as shown in Figure 2A. By selecting the bands shown in Figure 2B, it is possible to extract the ion mobility mass spectrum and export it into MassLynx Software for further interpretation, as shown in Figure 3.

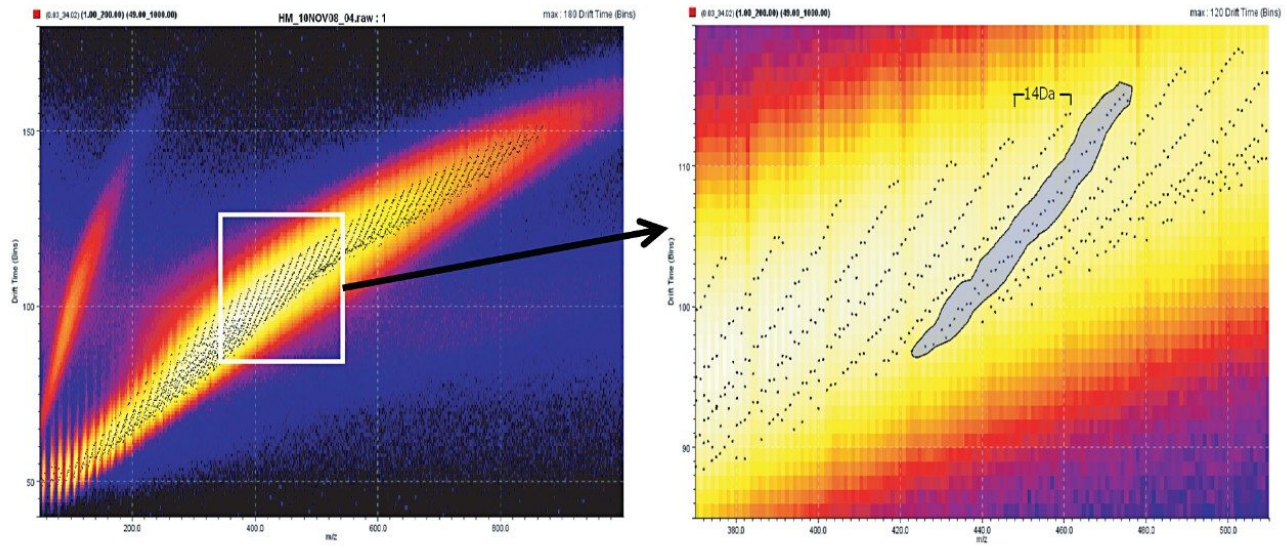

Figure 2A. View of the oil sample using DriftScope v.2.1.

Figure 2B. Expanded view for the oil sample showing bands, separated by ion mobility.

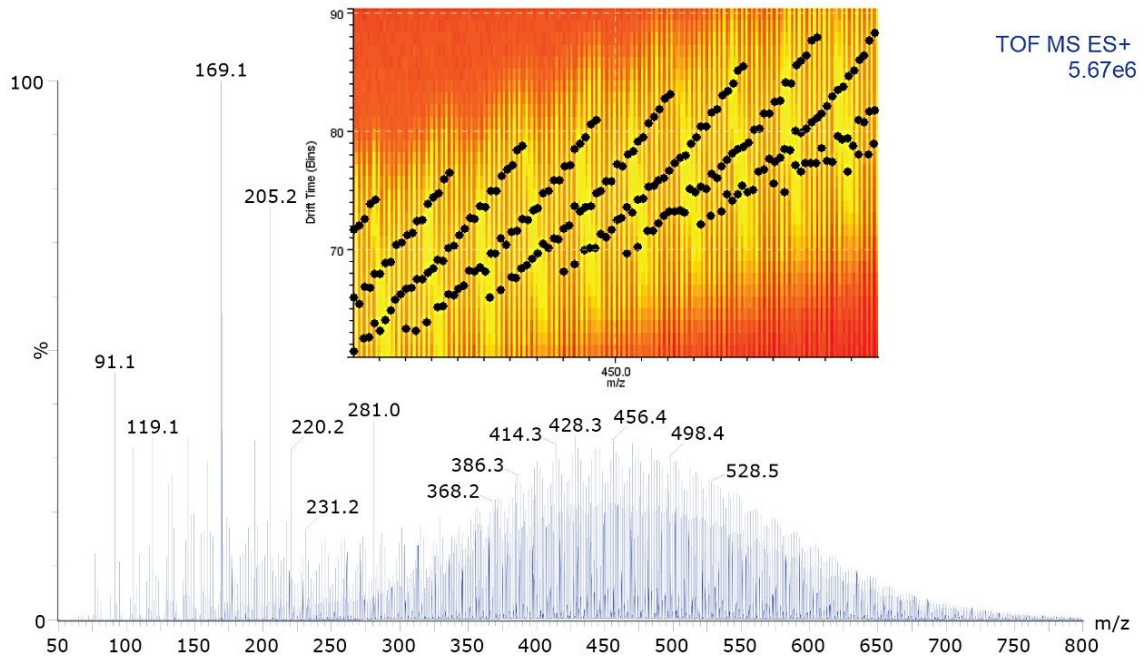

Figure 3. Ion mobility extracted spectrum of a selected homologous series from a crude oil sample.

Ion mobility separation (IMS) combined with direct ionization using the ASAP has previously been illustrated.[2] The orthogonality of IMS acts as an enabling technology where crude oil sample analysis can be performed with no prior chromatographic separation or sample preparation. The combination of ASAP-IMS-MS shows the potential for this technique to fingerprint crude oil samples, and offers a route to the analysis of involatiles, which cannot be achieved using GC-MS. Useful information was readily extracted from complex data using DriftScope Mobility Environment Software v.2.1.

Conclusion

- ASAP provides an easy and quick means to introduce a sample and produce screening data, without the constraints caused either by chromatographic conditions, or by ionization solvent compatibility.
- Ion mobility brings an additional dimension to the analysis of complex samples such as crude oil.

- The potential to separate isomers can simplify the mass spectra, and facilitates the characterization of complex samples.
- IMS-MS extends the capability of direct ionization techniques.

References

1. F A Fernandez-Lima, C Becker, A M McKenna, R P Rodgers, A G Marshall, and D H Russell. *Anal Chem*. 81: 9941–9947, 2009.
2. G Bondoux, H Major, M McCullagh. Petrochemicals Analysis using Novel Sources and Ion Mobility. Waters Corporation Poster (no. 720003712en). Presented at the Third EuCheMS Chemistry Congress, Nürnberg, Germany, September 2010.

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