

Using the Waters Atmospheric Solids Analysis Probe (ASAP) in an Walk-Up Environment

Waters Corporation

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief demonstrates the feasibility of the Atmospheric Solids Analysis Probe (ASAP) in a walk-up environment, organic synthesis reactions were monitored.

Benefits

Without reaction workup or sample preparation, in less than one minute, sample information can be obtained and informed decisions made without delay.

Introduction

In organic synthesis labs, reactions are often monitored by thin layer chromatography (TLC), which requires mobile phase optimization. Developing a TLC plate can be a time-consuming process, whereas all chemists need to accomplish is to monitor when the disappearance of the starting materials and the

appearance of the final product.

To increase the efficiency of the analysis of these reactions, an open access ASAP system was introduced. With minimal training, chemists were able to analyze their own samples while the analytical chemists concentrated on more difficult compounds.

Without reaction workup or sample preparation, in less than one minute, molecular weight information can be obtained and informed decisions made without delay.

Results and Discussion

ASAP coupled to an ACQUITY SQD was used for the analyses. The sampling procedure is shown in Figure 1. First, the sample was loaded onto the sealed glass melting point capillary tube of the ASAP probe by dipping the tip into the sample. The sample information was then entered into the OALogin software (Figure 2), which is a tool with MassLynx Software's OpenLynx Open Access Application Manager.



Figure 1. The sample is loaded directly onto the tip of a glass capillary. The sample is then directly inserted into the ionization source chamber. Bulk MS data are collected in seconds.

OALogin

Mode Security

Login Information

Your Name: Job ID:

Your Group: Description:

Methods:

ASAP	ESCI mass spectra (+). Scan range 100-2000.
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Sample Details

Number of Samples

SampleID	<input type="text" value="541564-54-02"/>	Mass1	<input type="text" value="149.1"/>
Mass2	<input type="text" value="260.3"/>	Mass3	<input type="text" value="391.4"/>

Press button to login samples. There are no Jobs waiting.
Available - 96 single shot locations

Figure 2. Single page OALogin window. After inserting probe into MS, users simply pick their name, choose an appropriate method, fill out details, and click Finish.

During the login procedure, a user is asked to enter in a minimal amount of data. On a single page, the user enters their name and chooses an appropriate method from a predefined list. They then enter sample information, place the probe in the outer assembly, and hit OK.

Once the ASAP probe was inserted into the sealed MS source enclosure, the desolvation gas was rapidly heated to 400 °C for MS acquisition. MS full scan data from 60 to 2000 amu was acquired for 0.5 min using a 0.2 sec scan duration. Target masses were extracted from the full scan data for reporting. The target masses were for the precursors and the final product.

The report was emailed to the user as a pdf (Figure 3). The report contained a simple table showing whether each target mass was found or not, as well as a spectra showing the found masses. The pdf format aided in copying the results to an electronic lab notebook. This facilitated viewing and sharing of the information.

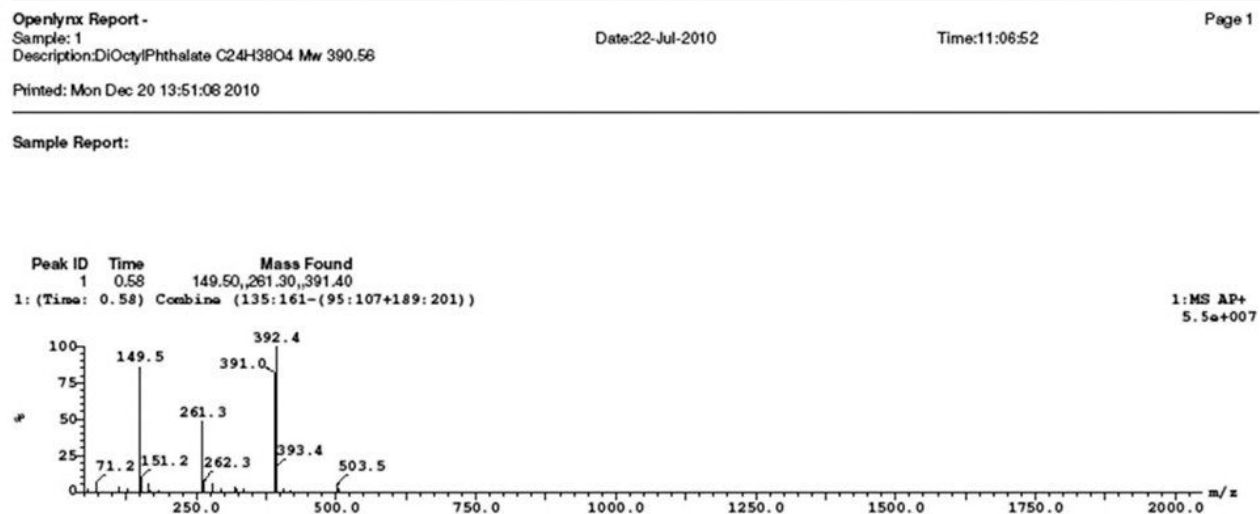


Figure 3. ASAP report emailed to user as a pdf upon completion of analysis. This report simply shows the spectra of the sample.

Conclusion

The ASAP probe can be used in conjunction with a quadrupole mass spectrometer to examine starting materials and monitoring the progress of reactions. Without reaction workup or sample preparation, in less than one minute, sample information can be obtained and informed decisions made without delay. Pairing ASAP with OALogin further simplifies the process and enables anyone to use the system.

As a result, the organic synthesis workflow efficiency is greatly enhanced, saving time and reducing the cost of analysis.

Featured Products

[Atmospheric Solids Analysis Probe <https://www.waters.com/10099674>](https://www.waters.com/10099674)

[OpenLynx Open Access <https://www.waters.com/10008851>](https://www.waters.com/10008851)

[MassLynx MS Software <https://www.waters.com/513662>](https://www.waters.com/513662)

[SQ Detector 2 <https://www.waters.com/134631584>](https://www.waters.com/134631584)

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