

Direct, Rapid Analysis of Orange Peel using the ASAP Ion Source



Objective

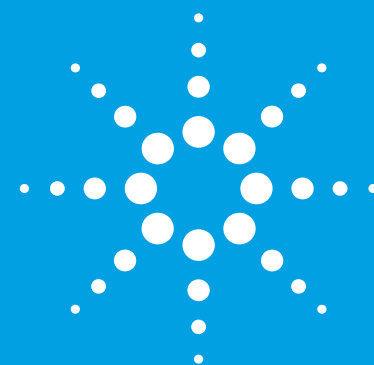
To directly and rapidly analyze contaminants from orange peel with high mass accuracy and resolution using an ambient desorption ionization technique, Atmospheric Solids Analysis Probe (ASAP), and an Agilent TOF or Q-TOF instrument.

Background

ASAP uses heated nitrogen to vaporize the sample and a corona discharge for ionization. The ion source is a modified APCI source with a corona needle and a probe for sample introduction. This source only takes a few minutes to set up and run.

This technique is fast, easy to use and does not require sample preparation. Using a high resolution instrument such as a TOF or a Q-TOF, it is possible to acquire high resolution accurate mass MS and MS/MS data in less than a minute.

This note describes the analysis of fungicides such as imazalil and thiabendazole from orange peel in less than 30 seconds without sample preparation using ASAP and an Agilent Q-TOF instrument.



Compounds

- Imazalil
- Thiabendazole

Key Benefits

- No sample preparation is needed with ASAP analysis
- Complex samples can be analyzed in less than 30 seconds using ASAP
- ASAP is fully compatible with Agilent TOF and Q-TOF instruments
- Typical mass accuracies for MS and MS/MS data are within 3 ppm



The Approach

The spectra shown below were acquired in less than 30 seconds following exposure of the sample in the ionization source. For ASAP analysis, a very small amount of sample can be placed in a sampling glass capillary. The capillary is then mounted onto a solids probe and introduced into the APCI source.

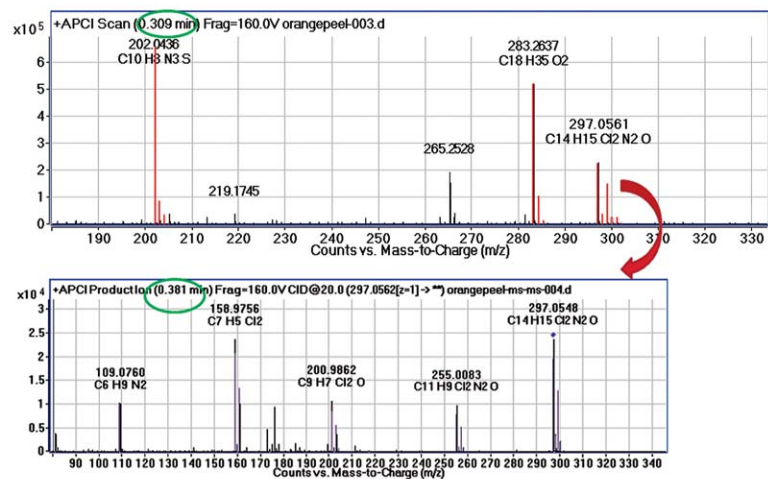
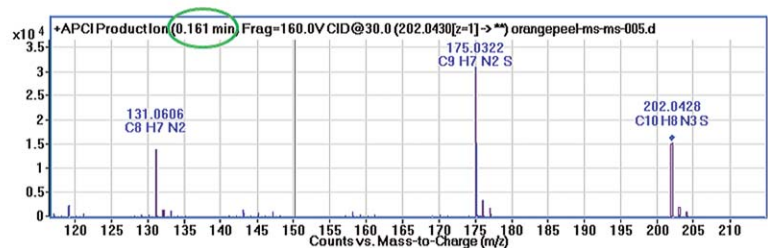


Figure 1. Orange peel scraped and analyzed with ASAP and an Agilent Q-TOF. The MS spectrum is shown in the top panel. Mass accuracy is within 2 ppm. The MS/MS spectrum of imazalil from orange peel is shown on the bottom panel. Mass accuracy is within 3 ppm. The data acquisition time of 0.3 min is circled in green in the top portion of the chromatogram.



MS Formula Results: • Product Ion (0.161 min) (202.0430 > *)

m/z	Ion	Formula	Abundance
131.0606	M ⁺	C ₈ H ₇ N ₂	13963.4
Best	Formula (M)	Ion Formula	Score
✓	C ₈ H ₇ N ₂	C ₈ H ₇ N ₂	99.41
Calc m/z	131.0604	Diff (ppm)	-1.35
Mass Match	99.91	Abund Match	98.12
DBE	6.5		
m/z	Ion	Formula	Abundance
175.0322	M ⁺	C ₉ H ₇ N ₂ S	31257.5
Best	Formula (M)	Ion Formula	Score
✓	C ₉ H ₇ N ₂ S	C ₉ H ₇ N ₂ S	96.89
Calc m/z	175.0324	Diff (ppm)	1.59
Mass Match	99.81	Abund Match	89.47
DBE	7.5		
m/z	Ion	Formula	Abundance
202.0428	M ⁺	C ₁₀ H ₈ N ₃ S	15440.1
Best	Formula (M)	Ion Formula	Score
✓	C ₁₀ H ₈ N ₃ S	C ₁₀ H ₈ N ₃ S	97.23
Calc m/z	202.0433	Diff (ppm)	2.74
Mass Match	99.28	Abund Match	94.44
DBE	8.5		

Figure 2. MS/MS spectrum of thiabendazole from orange peel with ASAP and an Agilent Q-TOF. The precursor ion peak at 202.0428 m/z and its fragments at 175.0322 m/z and 131.0606 m/z are shown. Mass accuracies are within 3 ppm. The data acquisition time of 0.16 min is circled in green in the top portion of the chromatogram.

Summary

ASAP can be used to rapidly analyze complex samples such as an orange peel directly without sample preparation. This ion source is fully compatible with Agilent TOF and Q-TOF instruments. Typical mass accuracies for MS and MS/MS data are within 3 ppm.

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