

Analysis of Simazine, Thiobencarb, and Thiuram by Liquid Chromatography/Mass Spectrometry Application

Environmental

Author

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Abstract

A liquid chromatography/mass spectrometry method using electrospray ionization in positive ion mode was successfully applied to the sensitive and simultaneous determination of the pesticides Simazine, Thiobencarb, and Thiuram.

Background

In recent years, the potential contamination of water supplies by runoff of many kinds of pesticides from golf courses and agricultural fields has become a societal problem. Many governments have established guidelines for pesticide use and water quality standards to limit such contamination. In Japan, the concentration limits in drinking water for the pesticides Simazine, Thiobencarb, and Thiuram are 3, 20, and 6 ppb, respectively.

Typically, gas chromatography-mass spectrometry (GC/MS) is used to determine Simazine and Thiobencarb in drinking water, while Thiuram is determined by high-performance liquid chromatography (HPLC) with ultraviolet (UV) detection. However, the Thiuram method used to date has problems with both selectivity and sensitivity. A better method of analysis is needed for this chemical. Such a method is described below.

Method

- Instrument: Agilent 1100 Liquid Chromatograph/Mass Spectrometer (LC/MS) with electrospray ionization (ESI) positive ion mode
Drying gas: N₂ (8 L/min, 350 °C)
Nebulizer: N₂ 40 psi
Fragmentor: 40 V (Thiuram), 70 V
Mass range: 100–500 amu

• LC Conditions:

Mobile phase A: CH₃OH/30 mM CH₃COONH₄ (50/50)
Mobile phase B: CH₃OH
Gradient: 0 % to 100 % B in 20 min
Flow rate: 0.2 mL/min
Oven temperature: 40 °C
Injection volume: 50 µL

- Column: Inertsil ODS3, 3.1 mm id × 250 mm long × 5 µm

Sample Analysis

All three pesticides were determined simultaneously using the Agilent 1100 LC/MS. The following figures illustrate both the sensitivity and applicability of this method.

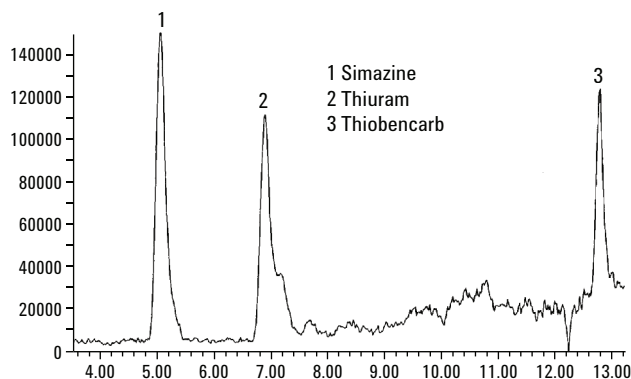


Figure 1. Total ion chromatogram of target pesticides, each at 5 ng.



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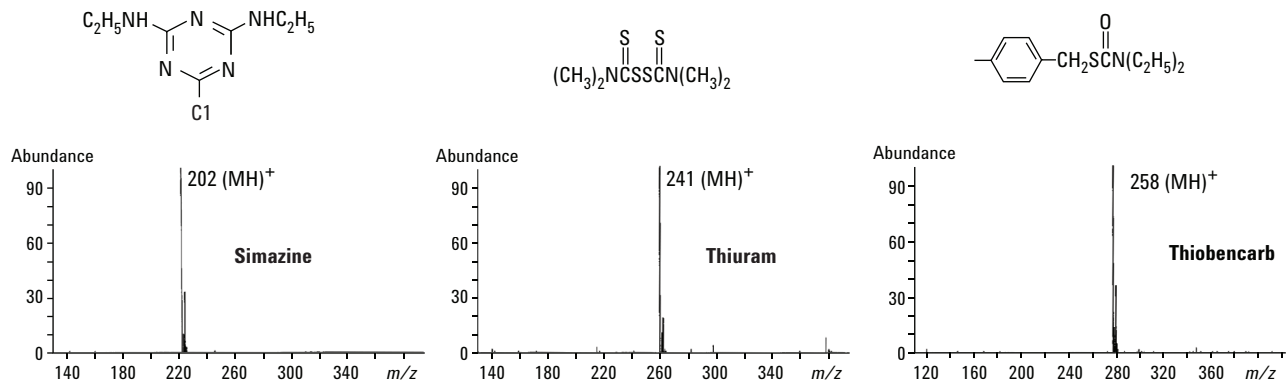


Figure 2. Mass spectra of target pesticides.

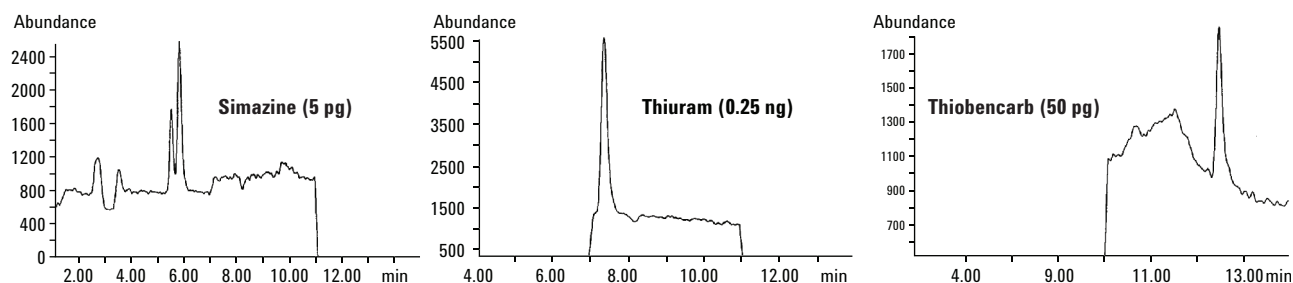


Figure 3. SIM chromatograms of target pesticides.

Conclusion

The LC/MS method described above is suitable for the simultaneous determination of the pesticides Simazine, Thiuram, and Thiobencarb. The peaks are well separated with detection limits of 0.02, 2.5, and 1 ppb, respectively, approximately 1/10 of the Japanese concentration limits.

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Printed in the USA
October 18, 2001
5988-4233EN



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