Application Note

Transferring Multiple Methods into a Single Analytical Solution Using Biocides in Consumer Products as a Model

Jane Cooper

Waters Corporation

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

Abstract

This application brief demonstrates to illustrate the simplicity of optimizing multiple methods for diverse biocides used in consumer products.

Benefits

The ACQUITY UPLC H-Class System enables a streamlined approach to multiple method analysis.

Introduction

Waters ACQUITY UPLC H-Class System offers the flexibility of the quaternary solvent pump, with the simplicity of flow-through needle injections.

With a wide range of UPLC column substrates and chemistries available, and the multi-solvent blending capabilities available with the ACQUITY UPLC H-Class System, additional scope both during method development and with routine analysis is now obtainable.

Biocides are chemical substances used in a wide range of products to either control or render safe harmful organisms. Various biocides are included in restricted substances lists (RSLs) utilized by many companies in order to protect their products for consumers, their workers, and also the community/environment.

This technology brief illustrates the flexibility users have with the ACQUITY UPLC H-Class System to combine biocide analytical suites of analyses and achieve high resolution, sensitivity, and throughput with sub-2-µm particle columns.

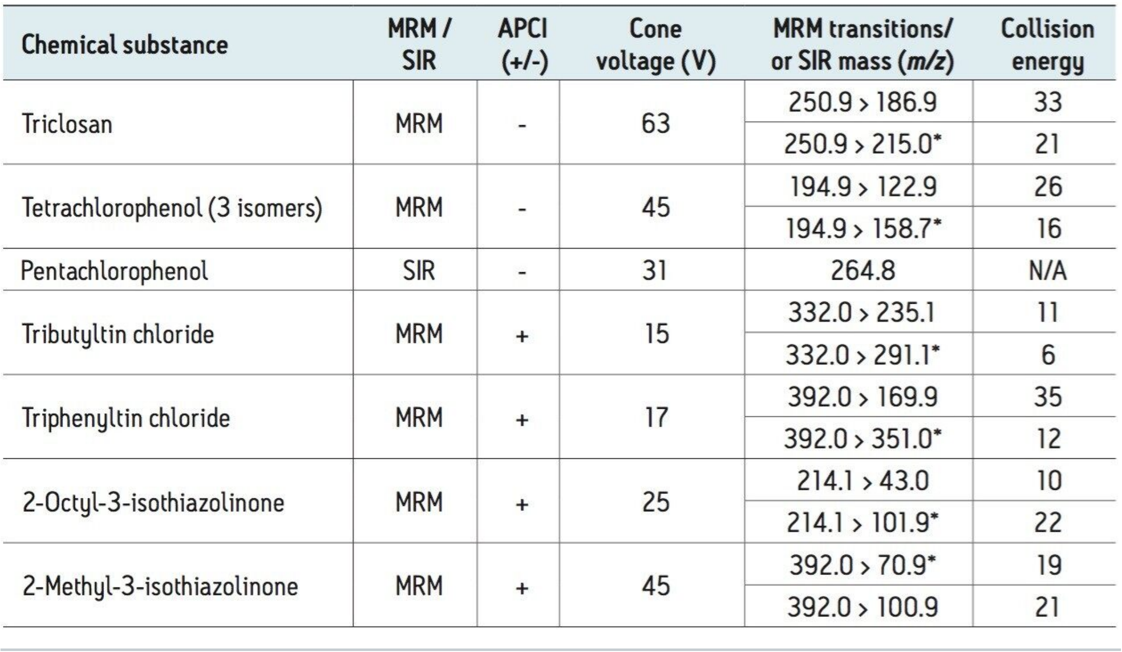
The scope to combine suites of analyses offers the chemical industry valuable time and cost savings, faster sample turnaround times, and an associated reduction in solvent usage.

Figure 1. ACQUITY UPLC H-Class System with Xevo TQD.

Results and Discussion

This investigation uses the Xevo TQD with atmospheric pressure chemical ionization (APCI), coupled to an ACQUITY UPLC H-Class System, for the detection of a range of biocide compound groups that would typically be analyzed using different chromatographic conditions.

Optimum multiple reaction monitoring (MRM) or selected ion recording (SIR) conditions were developed, as shown in Table 1.



Chemical substance	MRM / SIR	APCI (+/-)	Cone voltage (V)	MRM transitions/ or SIR mass (*m/z*)	Collision energy
Triclosan	MRM	-	63	250.9 > 186.9	33
				250.9 > 215.0*	21
Tetrachlorophenol (3 isomers)	MRM	-	45	194.9 > 122.9	26
				194.9 > 158.7*	16
Pentachlorophenol	SIR	-	31	264.8	N/A
Tributyltin chloride	MRM	+	15	332.0 > 235.1	11
				332.0 > 291.1*	6
Triphenyltin chloride	MRM	+	17	392.0 > 169.9	35
				392.0 > 351.0*	12
2-Octyl-3-isothiazolinone	MRM	+	25	214.1 > 43.0	10
				214.1 > 101.9*	22
2-Methyl-3-isothiazolinone	MRM	+	45	392.0 > 70.9*	19
				392.0 > 100.9	21

*Table 1. Biocides, ionization mode, cone voltages, MRM transitions or SIR mass, and associated collision energy values (*refers to the quantification transition).*

In order to optimize chromatographic separations, there are many important factors to consider including: LC system, detection method, choice of LC column, mobile phase(s), and mobile phase buffers. The choices of mobile phase buffers depend upon the compounds to be analyzed and the associated ionization mode used for detection. Buffers affect both the pH and the ionic strength of the mobile phase, and influence such factors as selectivity and peak shape.

Effects caused by the choice of mobile phase buffer with regard to the analysis of biocides are illustrated in Figure 2. The three tetrachlorophenol isomers were resolved when the basic ammonium acetate (AA) buffer was used, but the peak shape of the tin compounds, shown in Figure 2a, was very poor. The three tetrachlorophenol isomers were not resolved, however, when the acidic formic acid (FA) buffer was used, while the peak shape of the tin compounds, shown in Figure 2b, was markedly improved.

Typically, to achieve improved resolution of the three tetrachlorophenol isomers, improved selectivity, and peak shape of the tin compounds, two separate LC methods would be required; one using an acidic buffer, and the other using a basic buffer. Using the quaternary pump of the ACQUITY UPLC H-Class System, this can all be achieved in one UPLC method, shown in Figure 2c, by swapping the choice of buffer during the run.

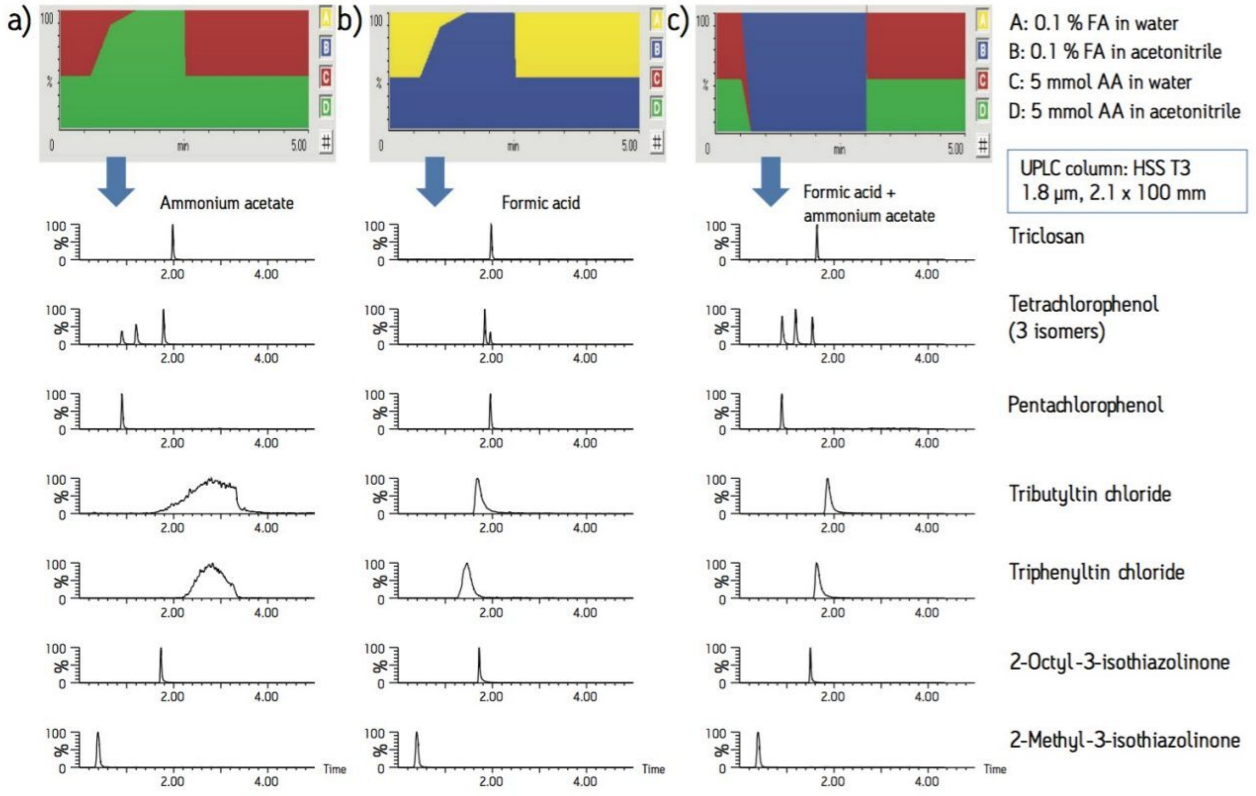


Figure 2. MRM/SIR chromatograms for select biocides compounds in a mixed solvent standard using different mobile phase buffer: 2a. ammonium acetate, 2b. formic acid; and 2c. a combination of ammonium acetate and formic acid.

Combining methods offer time and cost savings, enabling greater sample throughput and reduced solvent consumption. Also reducing the amount of LC methods required saves time spent on switching and equilibrating LC methods in between different analytical suites of analyses.

Conclusion

The flexibility offered using the quaternary solvent pump of the ACQUITY UPLC H-Class System expands the benefits of UPLC technology. It provides improved scope for method development and multi-method analyses, while maintaining high resolution, sensitivity, and throughput offered by sub-2-µm particle columns.

The scope to combine suites of analyses offers the chemical industry valuable time and cost savings, faster sample turnaround times, and an associated reduction in solvent usage.

Featured Products

ACQUITY UPLC H-Class PLUS System <https://www.waters.com/10138533>

Xevo TQD Triple Quadrupole Mass Spectrometry <https://www.waters.com/134608730>

720004609, February 2013