

The example data presented here represents typical expected performance and is provided for the purposes of illustration and user guidance only. All Waters analytical instruments are installed and tested in accordance with Waters Standard Performance Tests. In presenting these data no agreement is implied by Waters to perform any additional non-standard performance tests during the installation.

XEVO TQ-XS UPLC/MRM

System Sensitivity – Positive Ion ESI

Simultaneous MRM / RADAR acquisition

This document presents example data based on monitoring the UPLC MRM response for injections of a pesticide mix whilst simultaneously performing a RADAR acquisition. Please see the relevant document for a full listing of the Xevo TQ-XS performance specifications.

EXPERIMENTAL CONDITIONS

Sample

Test sample: 10 pg/μL pesticide mix (in 90% water: 10% acetonitrile)

LC Conditions

Instrument: ACQUITY I-Class
Column: ACQUITY BEH, 100mm x 2.1mm, 1.7μm
Injection volume: 10 μL
Flow rate: 0.45 mL/min
Mobile phase A: water + 10 mL of 1M ammonium acetate
Mobile phase B: methanol + 10 mL of 1M ammonium acetate
Sample Manager Wash: acetonitrile
Purge syringe: 90% water, 10% methanol
Seal Wash: 90% water, 10% methanol
Column Temp: 45°C
Sample Temp: 4°C

UPLC Gradient

Time (min)	%A	%B	Curve
0.00	98	2	-
0.25	98	2	6
12.25	1	99	6
13.00	1	99	6
13.01	98	2	6
17.00	98	2	6

MS Conditions

Instrument: Xevo TQ-XS
Ionization mode: ESI positive
Resolution: Peak width at half-height of precursor and product ions <1 Da
MRM spike rejection: Enabled
RADAR: 0.05s scan time, 50 – 550 Da mass range.
MRM: m/z 230 > 174.

Software

MassLynx: V4.2, SCN943

RESULTS

Figure 1 shows a UPLC MRM chromatogram obtained whilst acquiring a MRM and RADAR scan. The example shows the two peaks, Sethbutylazine at 8.12 min and Tertbutylazine at 8.36 min.

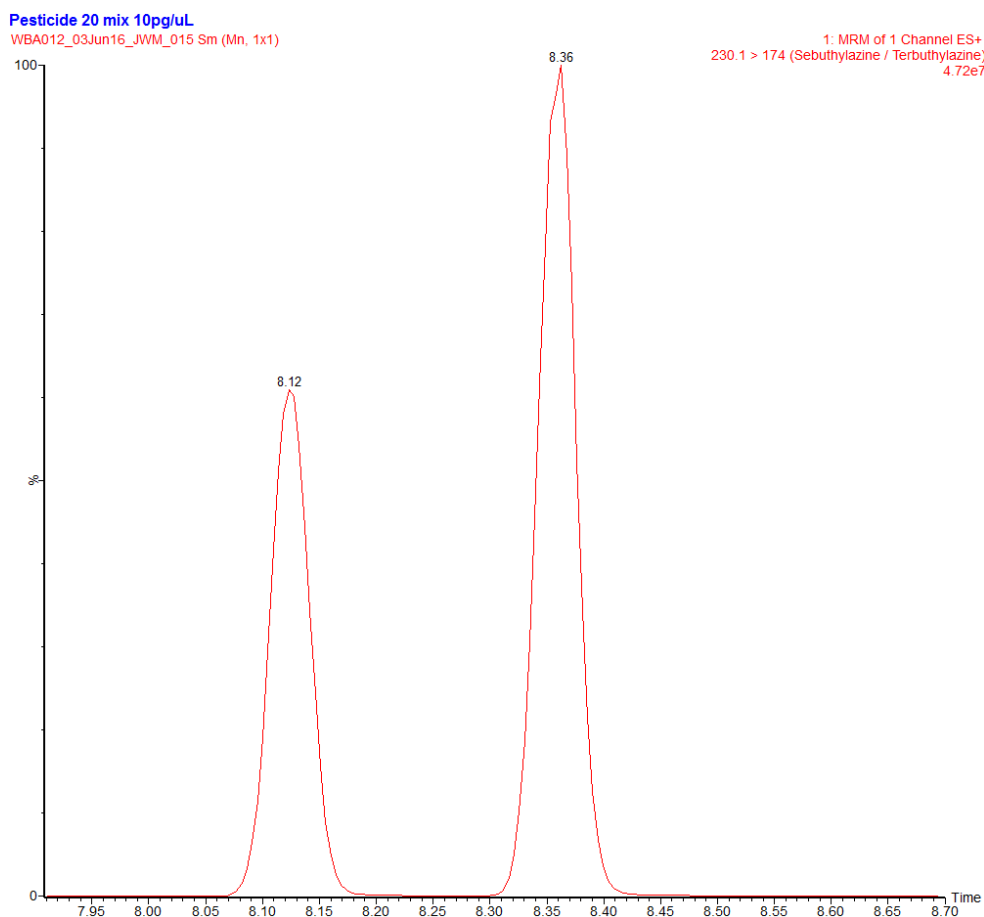


Figure 1.

10pg/ μ L Sethbutylazine and Tertbutylazine (100pg on column), MRM (m/z 230.1 > 174)

Figure 2 shows the RADAR scan chromatogram obtained whilst simultaneously acquiring the MRM shown in figure 1. The example shows the two peaks, Sethbutylazine at 8.12 min and Tertbutylazine at 8.36 min. A further peak with precursor m/z 230 was also discovered at 5.54 minutes. Without the RADAR scan this peak may have remained undiscovered.

Pesticide 20 mix 10pg/uL

WBA012_03Jun16_JWM_015 Sm (Mn, 1x1)

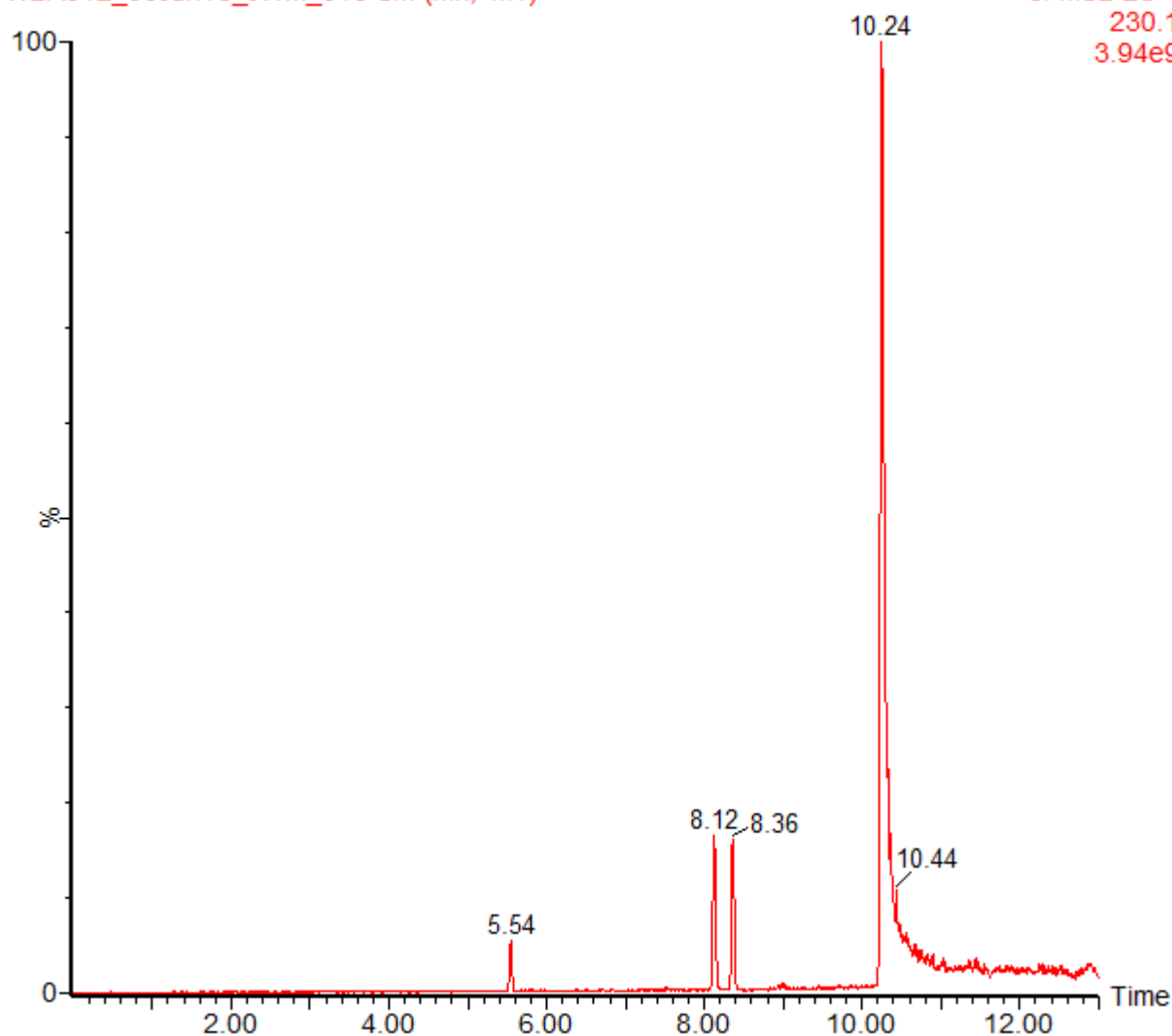
5: MS2 ES+
230.1
3.94e9

Figure 2.
The simultaneous RADAR scan (MS2 scan)

Figure 3 show the mass spectrum taken around 8.36 minutes. As expected the m/z value associated with Sethbutylazine dominates the image.

Pesticide 20 mix 10pg/uL

WBA012_03Jun16_JWM_015 1941 (8.353) Sm (Mn, 1x1.00)

5: MS2 ES+
5.30e7

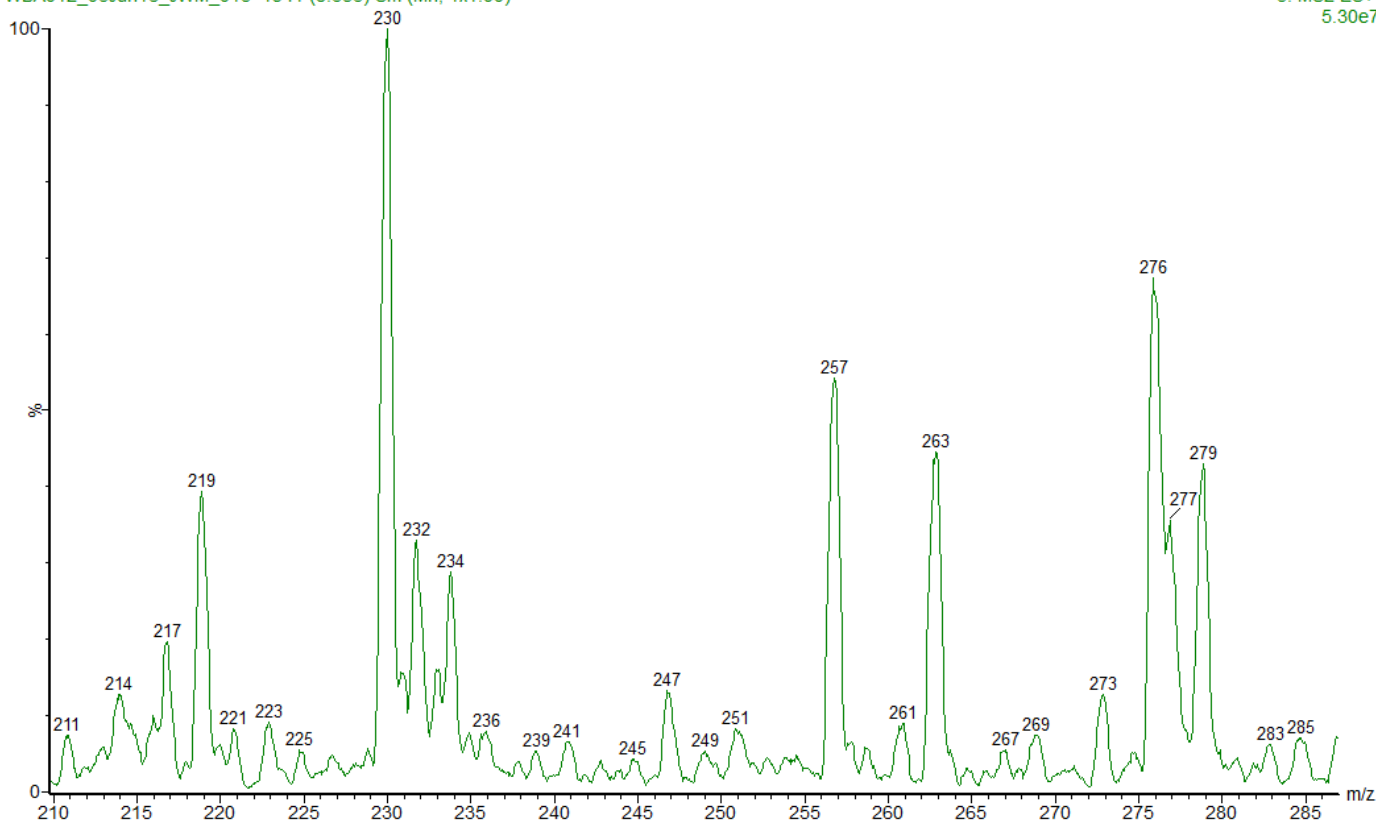


Figure 3.

Spectrum taken at 8.36 minutes. The largest peak is m/z 230 (Sethbutylazine)



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