

Acquity I-class TQ-XS Demo sample analysis report

-- *Group 3: Marine Biotoxins List A*

Introduction

AVA has provided us with four groups of samples.

- Group -1 : Sudan Dyes
 - Group -2 : Sweeteners
 - Group -3 :Marine Biotoxins List A
 - Group -4 :Marine Biotoxins List B
-
- This system must be able to run a variety of applications, including a sensitive assay for all the group of compounds mentioned in the above samples.
 - This report demonstrates the potential for the I-Class FTN/XEVO TQ-S to provide a robust and sensitive results for the above mentioned compounds.
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Executive Summary

- Nine marine biotoxins were detected in 0.25 ppb neat solution standard

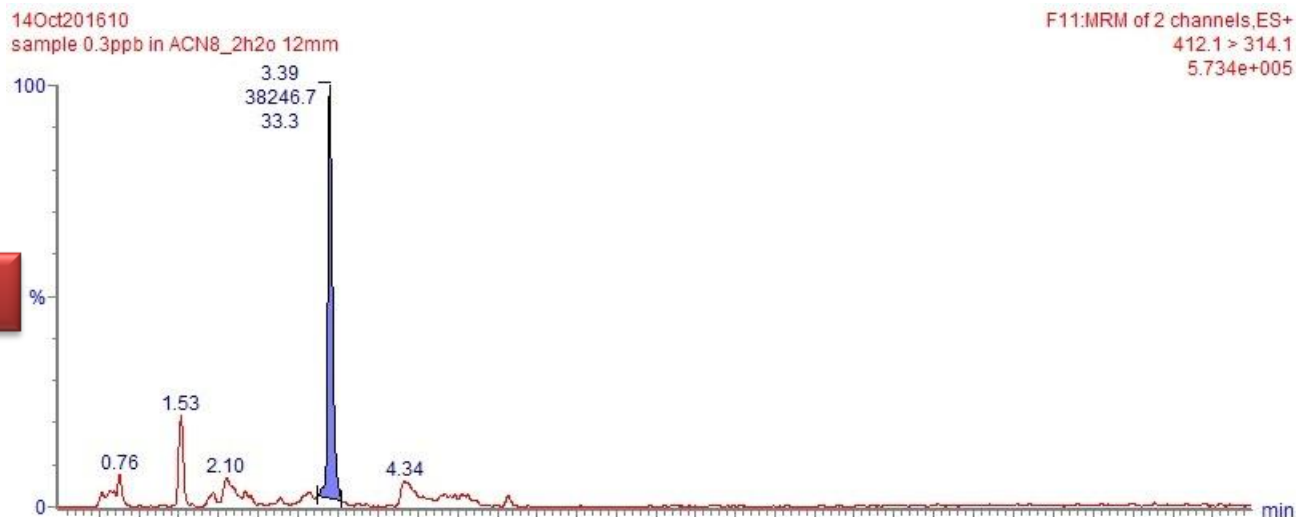
The background features a light green to yellow gradient. Overlaid on this are thin, light green circuit-like lines that meander across the upper portion of the image. The lower portion is filled with a pattern of small, semi-transparent white and yellow dots, creating a textured, grid-like appearance. A large, semi-transparent white geometric shape, resembling a stylized 'A' or a large triangle, is positioned behind the text.

Results

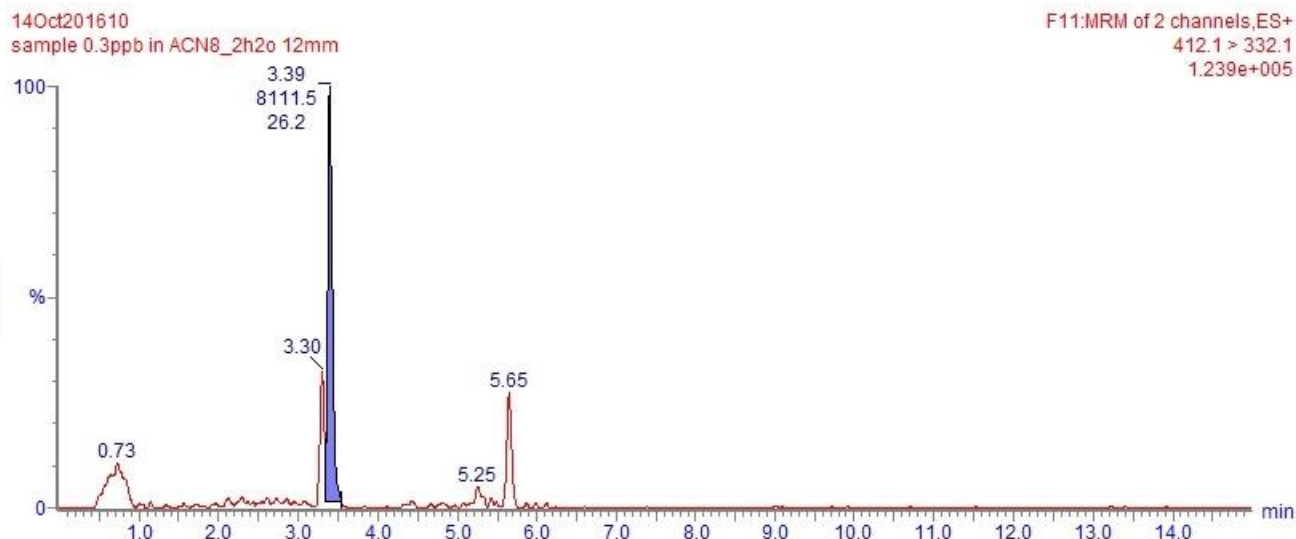
Chromatogram of **C4** at 0.25 ppb in Neat Solvent

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Quantifier Ion



Qualifier Ion

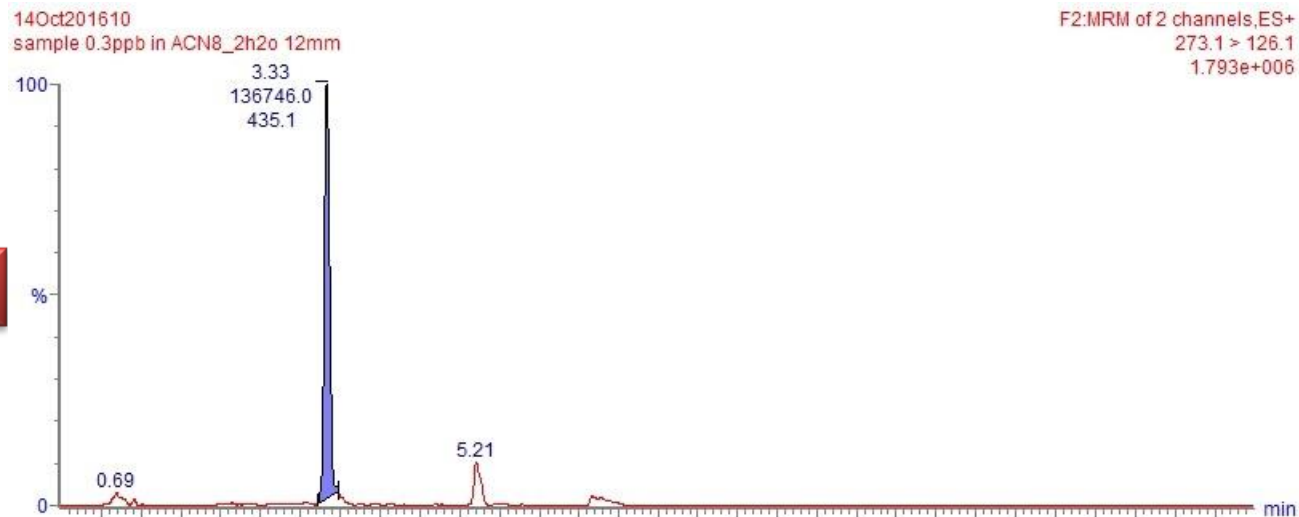


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

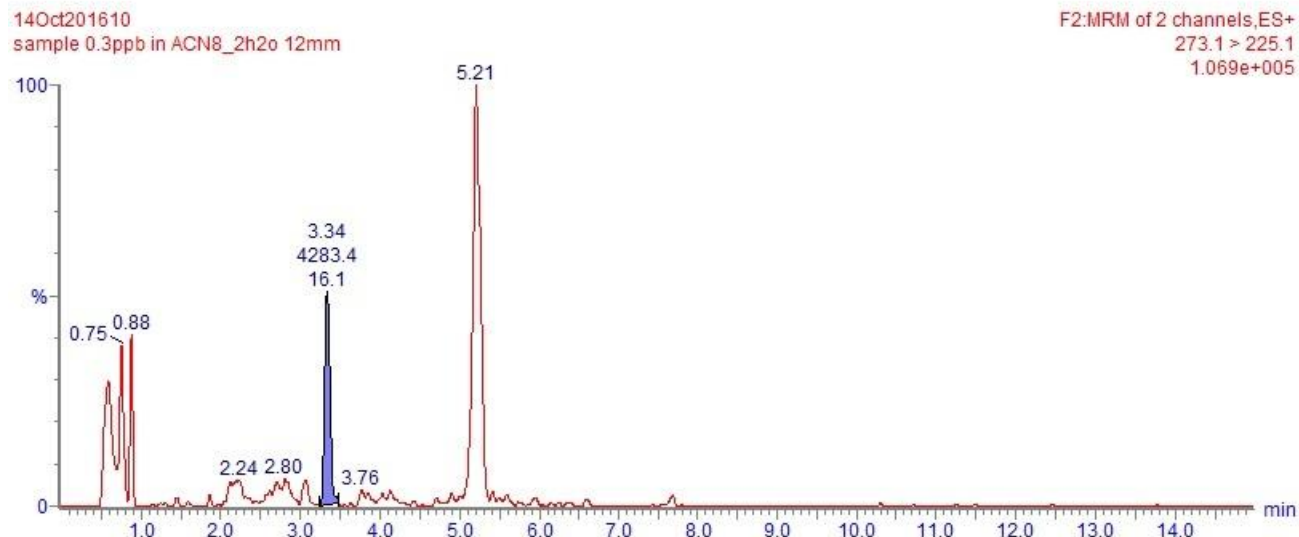
Chromatogram of *dc-NEO* at 0.25 ppb in Neat Solvent

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Quantifier Ion



Qualifier Ion

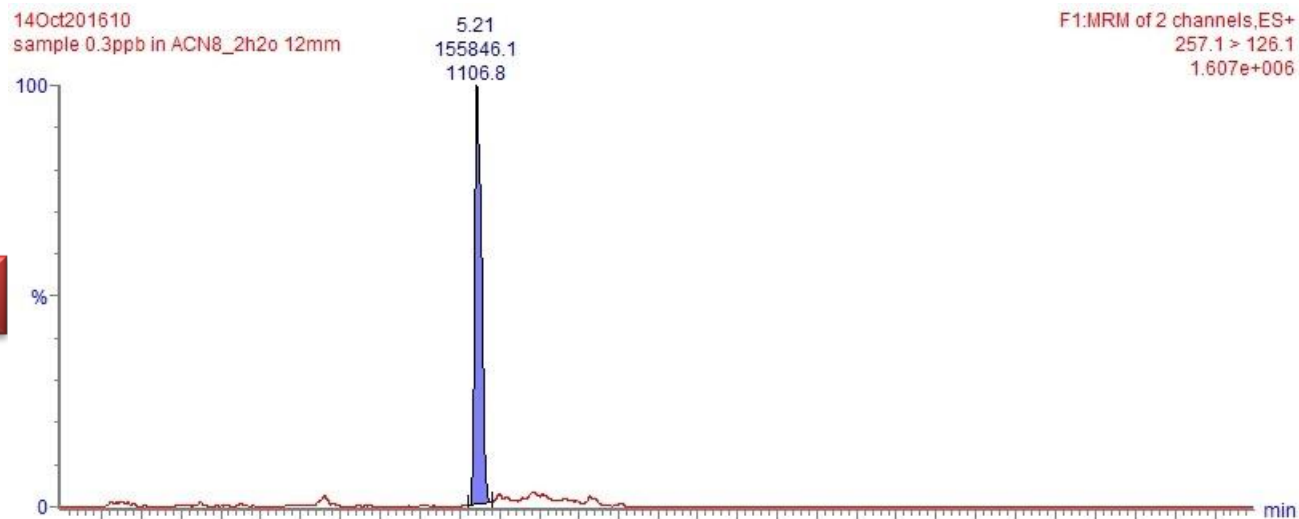


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

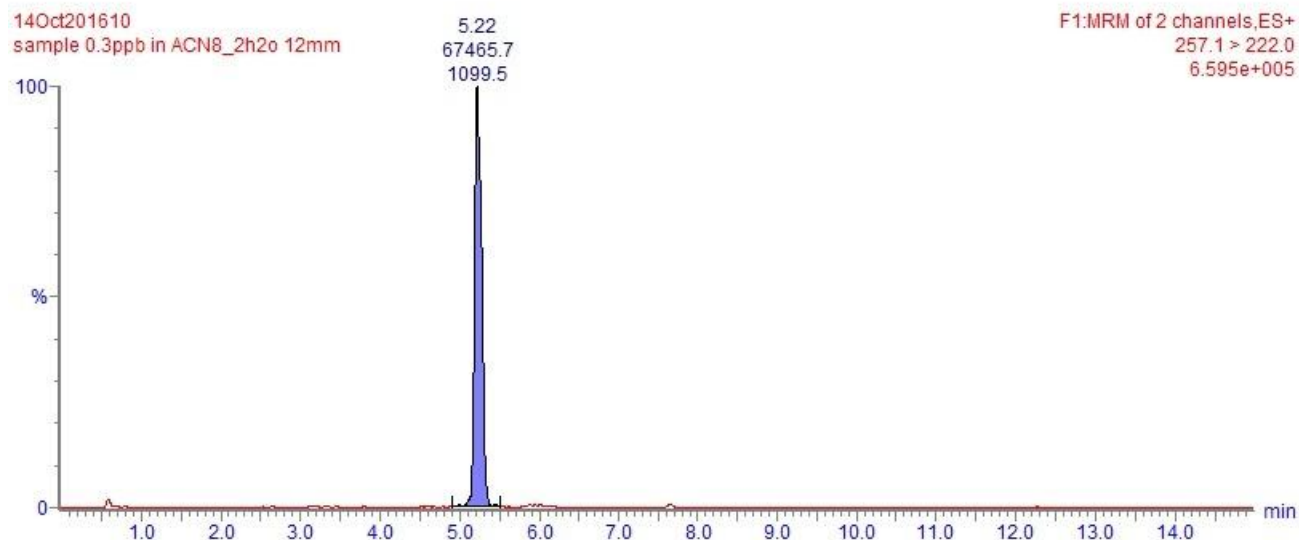
Chromatogram of *dc-STX* at 0.25 ppb in Neat Solvent

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Qualifier Ion

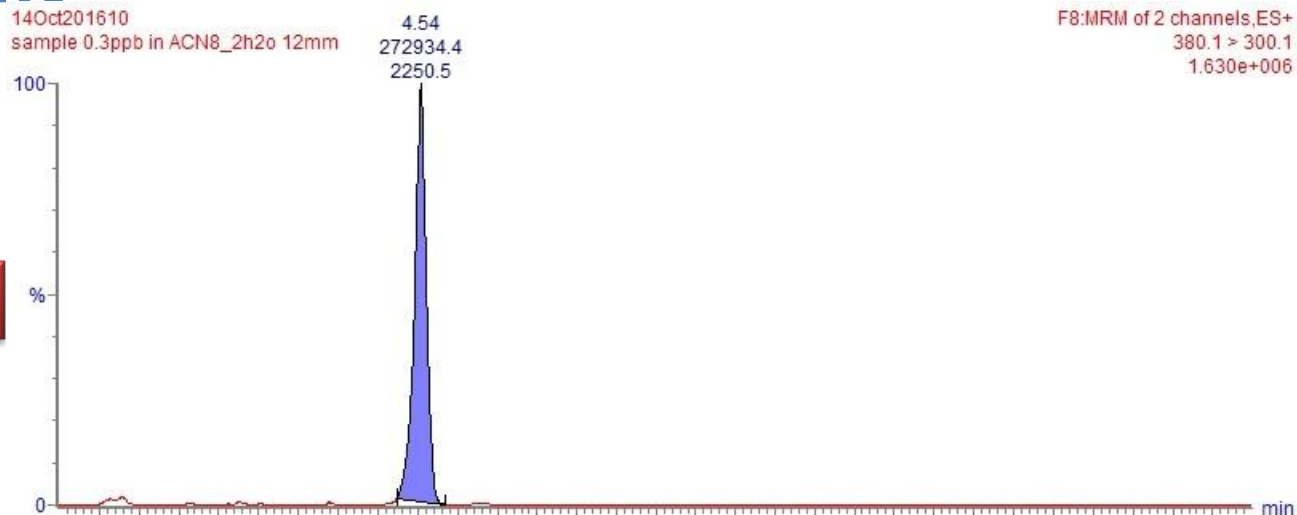


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

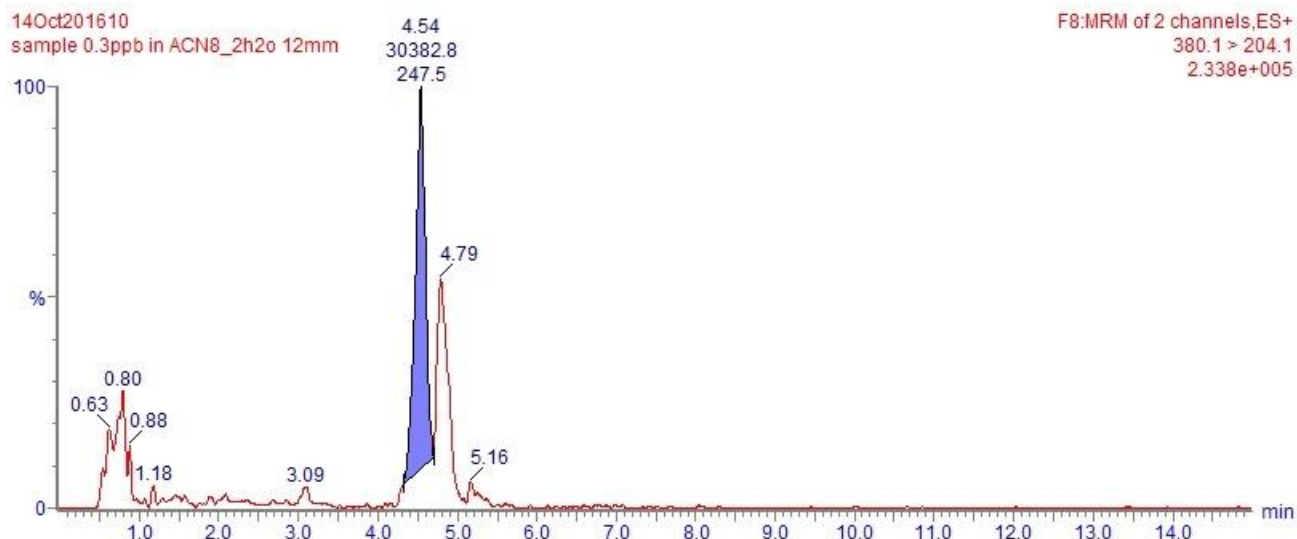
Chromatogram of **GTX5** at 0.25 ppb in Neat Solvent

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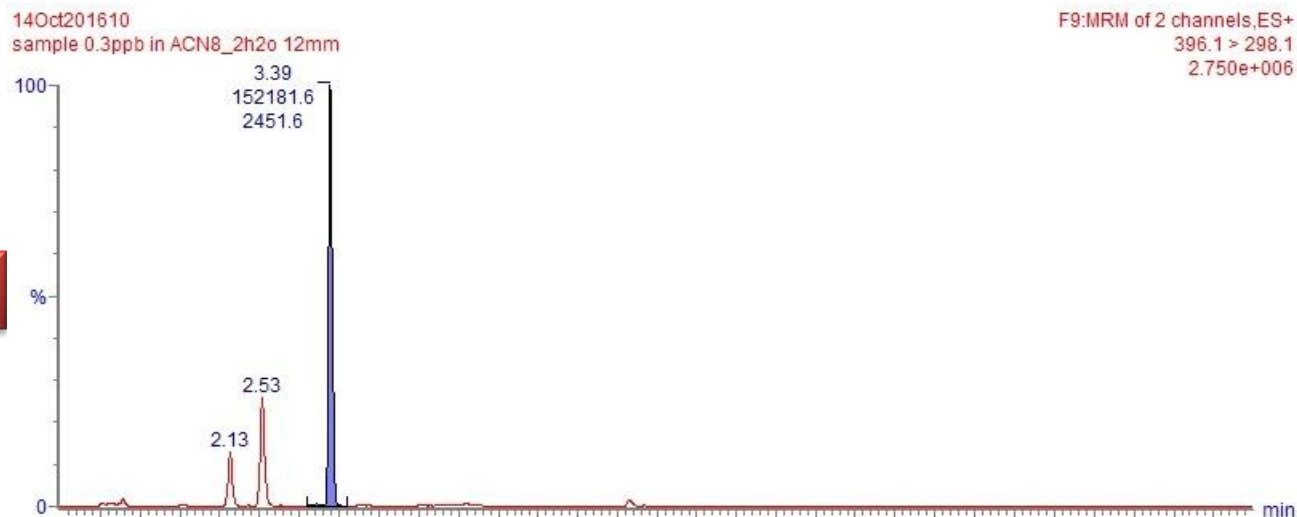


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

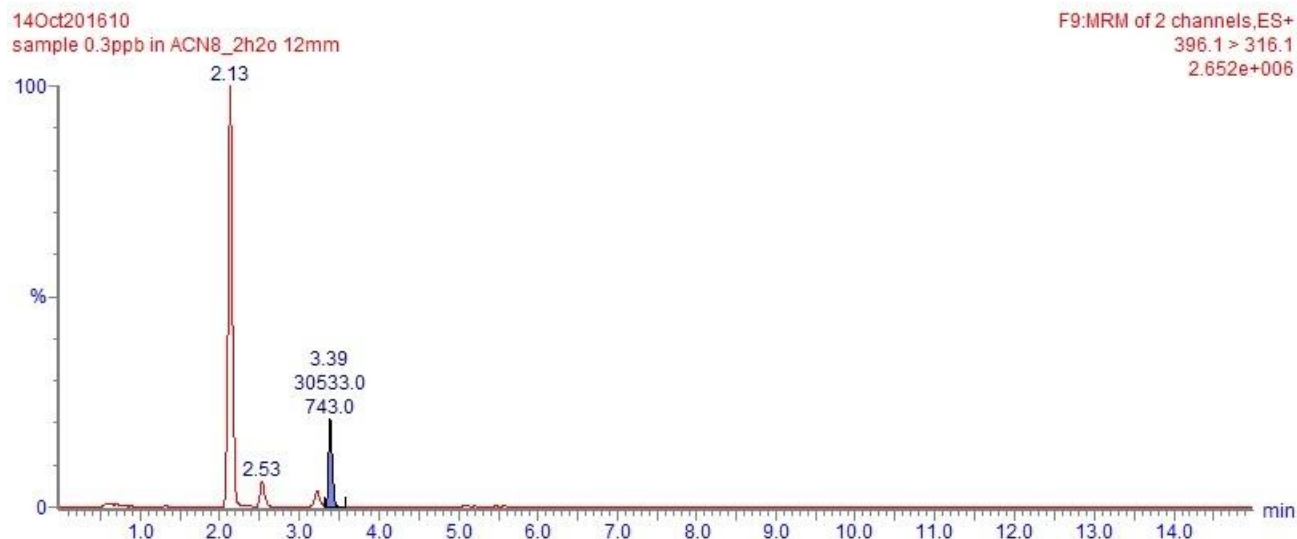
Chromatogram of **GTX6** at 0.25 ppb in Neat Solvent

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Qualifier Ion

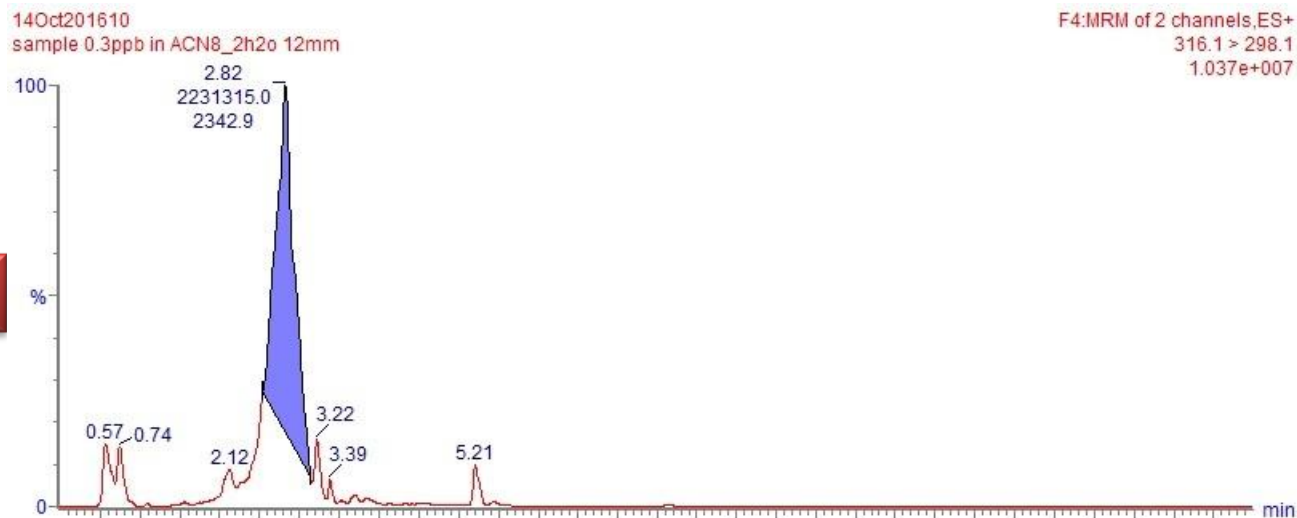


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

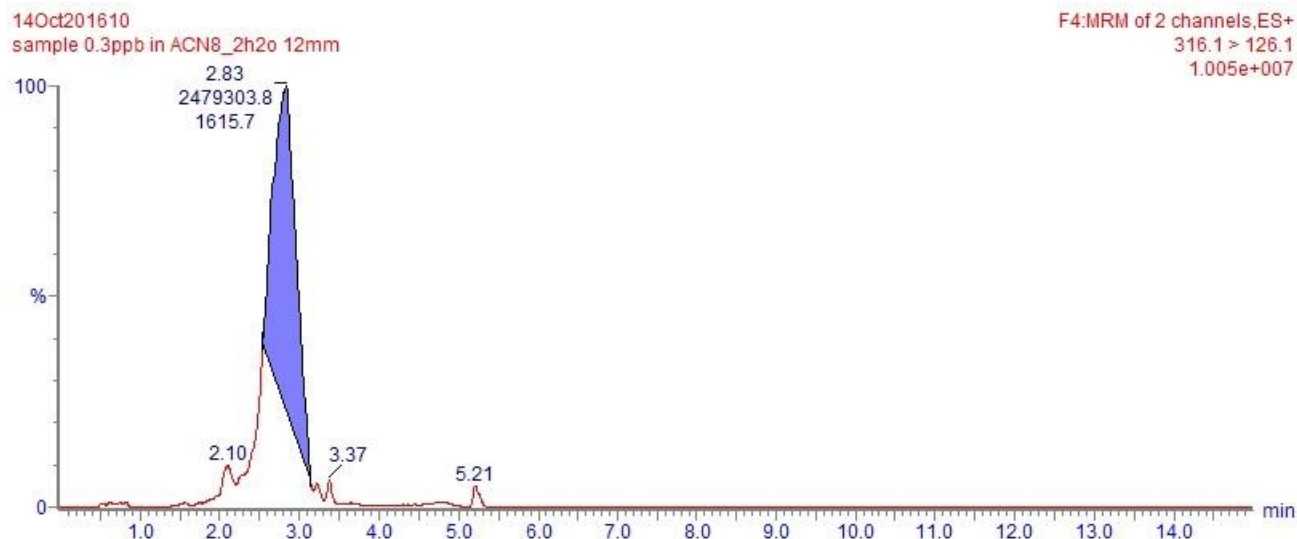
Chromatogram of **NEO** at 0.25 ppb in Neat Solvent

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Quantifier Ion



Qualifier Ion

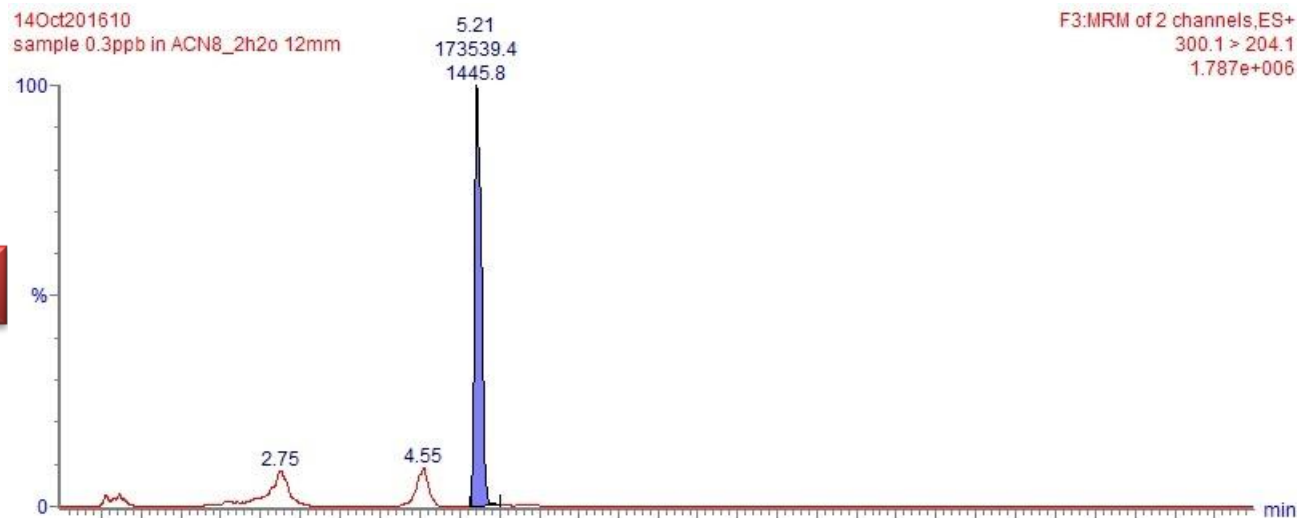


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

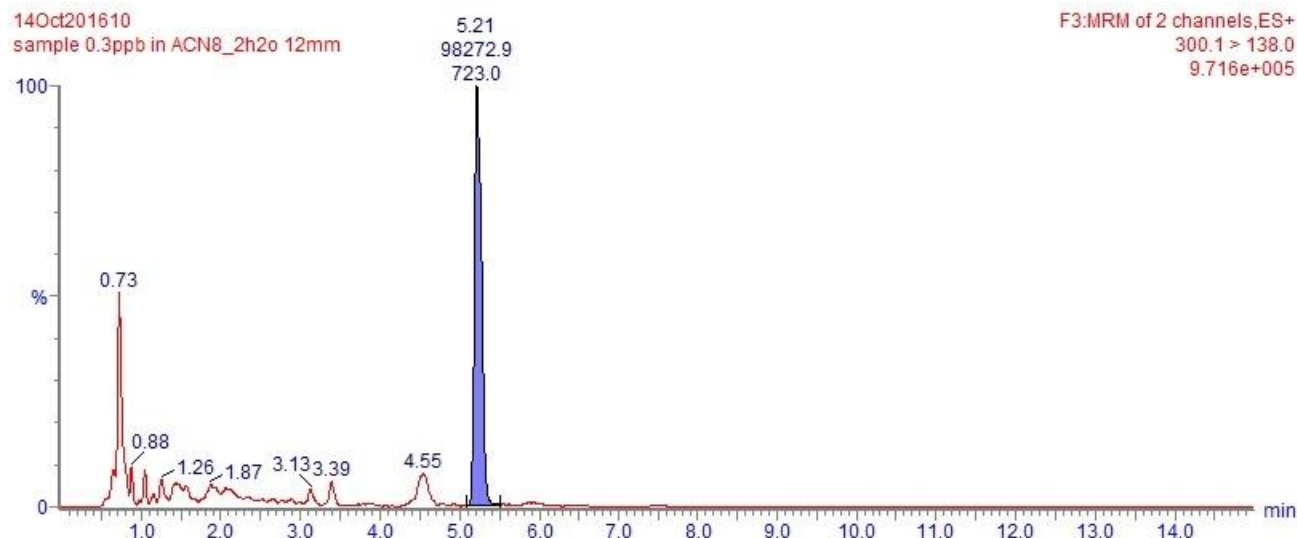
Chromatogram of **STX** at 0.25 ppb in Neat Solvent

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Quantifier Ion



Qualifier Ion

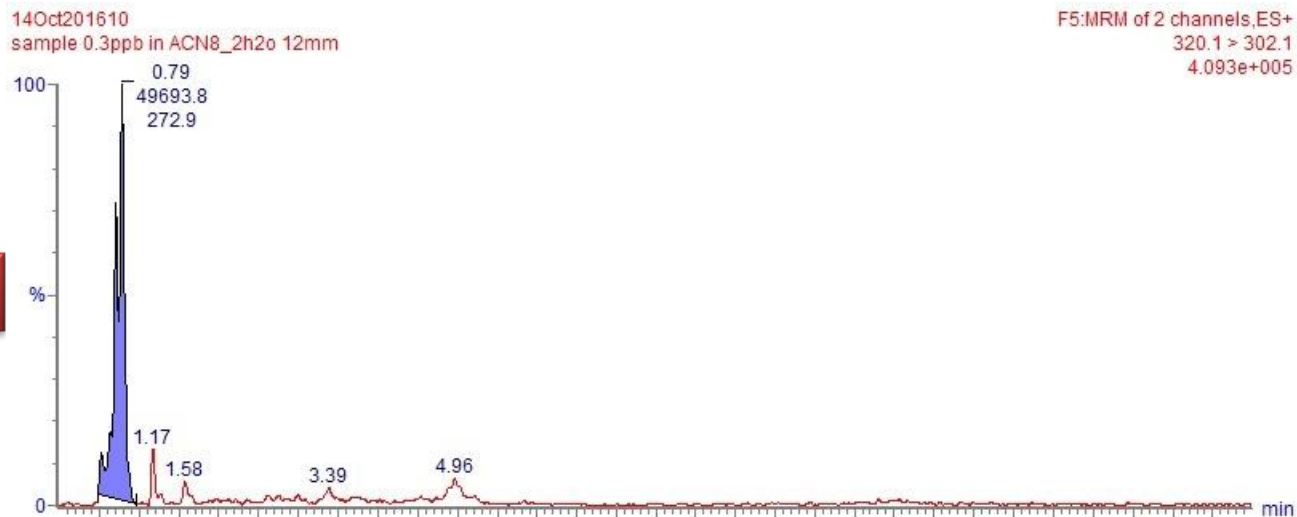


The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

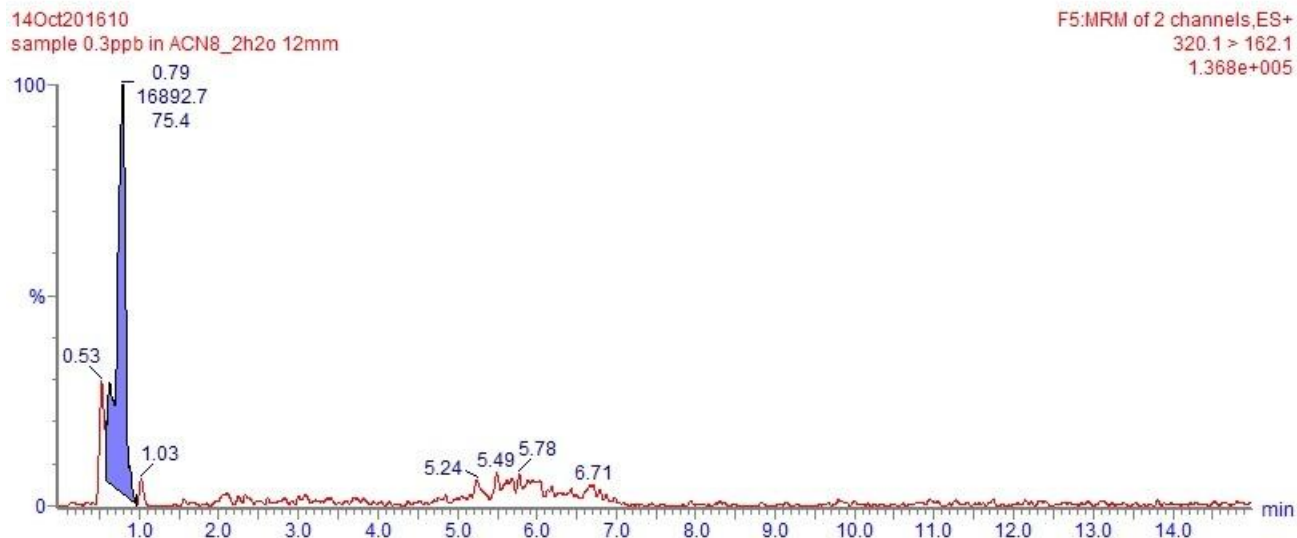
Chromatogram of **TTX** at 0.25 ppb in Neat Solvent

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Quantifier Ion



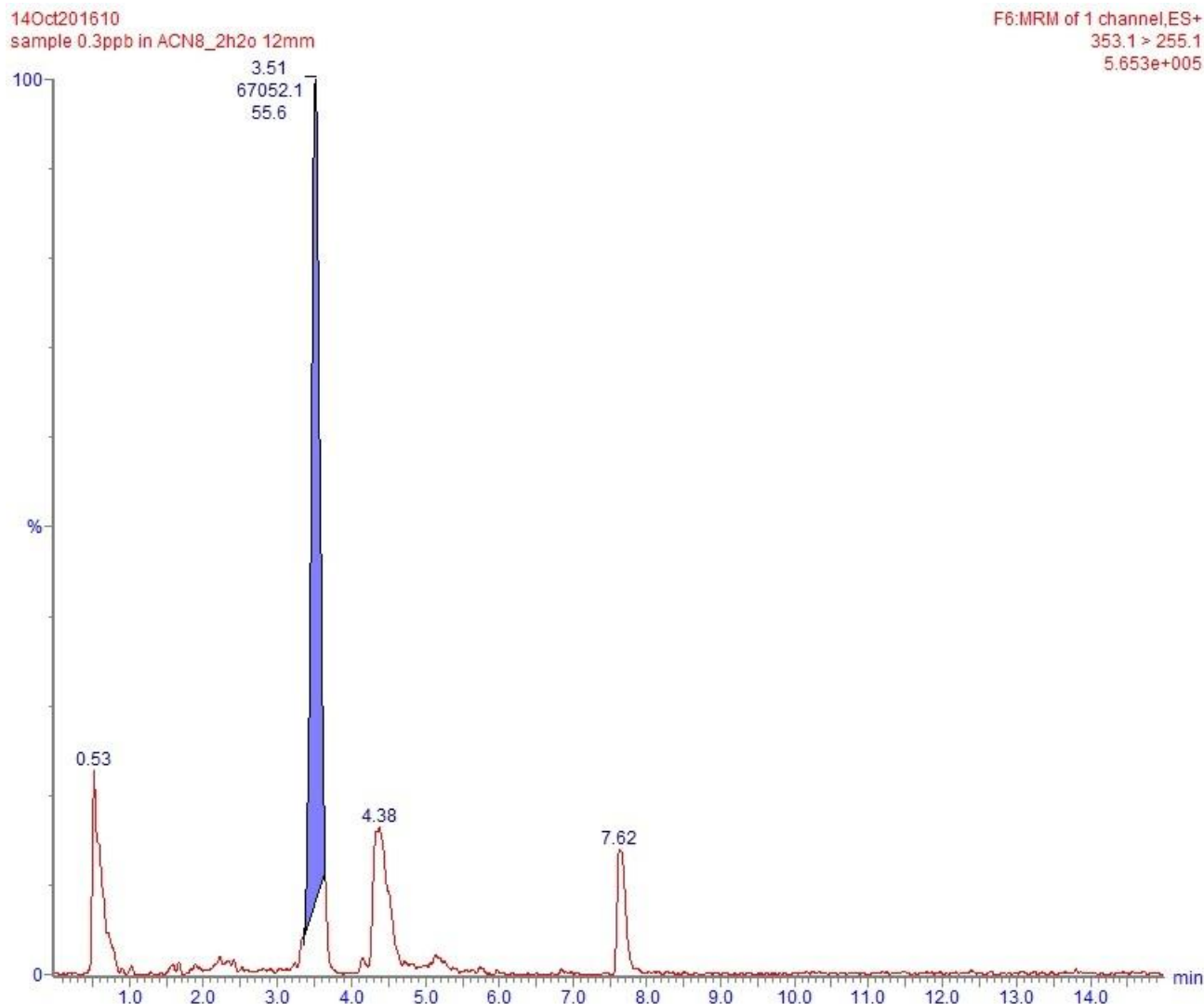
Qualifier Ion



The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram

Chromatogram of *dc-GTX3* at 0.25 ppb in Waters Neat Solvent

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The retention time (RT), peak response area, and peak signal-to-noise are shown on peak top of the chromatogram



Method

UPLC Conditions: I-Class

System	ACQUITY UPLC™ I-Class
Column	ACQUITY BEH Amide 100 mm x 2.1 mm, 1.7 µm
Column temperature	40°C
Flow	0.4 mL/min
Mobile phase	(A) Water/Formic Acid/NH4OH (500:0.075:0.3 v/v/v)
	(B) Acetonitrile/water/Formic acid (700:300:0.1 v/v/v)
Injection Vol (FTN)	10 µl



Time (min)	% A	% B
0.00	1	99
4.00	1	99
7.50	50	50
9.00	50	50
9.50	1	99
15.00	1	99

MS Conditions: Xevo TQ-XS

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Ionization Mode	ESI+, ESI-
Capillary voltage	0.5 kV (ESI+) & 0.5 kV (ESI-)
Source Temperature	150 °C
Desolvation Temperature	550 °C
Desolvation Gas Flow (L/Hr)	950



Xevo TQ-XS

MRM Transitions Based on Literature

Analyte	Parent (m/z)	Daughter (m/z)	Dwell (s)	Cone Voltage (V)	Collision energy (eV)	Mode of Ionization
C1	474.1	351.1	0.006	10	25	ES-
C1	474.1	122.0	0.006	10	30	ES-
C2	396.1	298.1	0.006	10	20	ES-
C2	396.1	298.1	0.006	18	20	ES+
C2	396.1	220.0	0.006	20	30	ES+
C2	396.1	316	0.006	20	10	ES+
C3	490.10	410.1	0.006	10	20	ES-
C3	490.10	392.1	0.006	10	20	ES-
C3	490.10	122.1	0.006	10	25	ES-
C4	412.1	314.1	0.006	10	20	ES-
C4	412.1	332.1	0.006	10	16	ES-

MRM Transitions Based on Literature (Continued)

Analyte	Parent (m/z)	Daughter (m/z)	Dwell (s)	Cone Voltage (V)	Collision energy (eV)	Mode of Ionization
dc-GTX1	367.1	274.1	0.006	10	20	ES-
dc-GTX1	367.1	349.1	0.006	10	17	ES-
dc-GTX1	367.1	289.1	0.006	10	19	ES-
dc-GTX2	351.1	164.0	0.006	10	30	ES-
dc-GTX2	351.1	333.1	0.006	10	17	ES-
dc-GTX2	351.1	273.1	0.006	10	10	ES-
dc-GTX3	351.1	255.1	0.006	10	18	ES+
dc-GTX3	351.1	273.1	0.006	10	17	ES+
dc-GTX4	369.1	271.1	0.006	10	18	ES+
dc-GTX4	369.1	289.1	0.006	10	18	ES+
dc-NEO	273.1	126.1	0.006	10	20	ES+
dc-NEO	273.1	225.1	0.006	10	18	ES+
dc-NEO	273.1	255.1	0.006	10	16	ES+
dc-STX	257.1	126.1	0.006	10	19	ES+
dc-STX	257.1	222.0	0.006	10	22	ES+
dc-STX	257.1	239.0	0.006	10	21	ES+

MRM Transitions Based on Literature (Continued)

Analyte	Parent (m/z)	Daughter (m/z)	Dwell (s)	Cone Voltage (V)	Collision energy (eV)	Mode of Ionization
GTX1	410.1	349.1	0.006	10	22	ES-
GTX1	367.1	367.1	0.006	10	15	ES-
GTX2	394.1	333.1	0.006	10	22	ES-
GTX2	394.1	351.1	0.006	10	16	ES-
GTX3	394.1	333.1	0.006	10	22	ES+
GTX3	394.1	351.1	0.006	10	16	ES+
GTX4	410.1	367.1	0.006	10	15	ES-
GTX4	410.1	349.1	0.006	10	22	ES-
GTX5	380.1	300.1	0.006	10	26	ES+
GTX5	380.1	204.1	0.006	10	16	ES+
GTX6	396.1	298.1	0.006	10	22	ES+
GTX6	396.1	316.1	0.006	10	15	ES+
GTX6	396.1	220.1	0.006	10	30	ES+

MRM Transitions Based on Literature (Continued)

Analyte	Parent (m/z)	Daughter (m/z)	Dwell (s)	Cone Voltage (V)	Collision energy (eV)	Mode of Ionization
NEO	316.1	298.1	0.006	10	15	ES+
NEO	316.1	126.1	0.006	10	26	ES+
NEO	316.1	220.1	0.006	10	24	ES+
STX	300.1	204.1	0.006	10	24	ES+
STX	300.1	138.0	0.006	10	30	ES+
STX	300.1	282.0	0.006	10	15	ES+
TTX	320.1	302.1	0.006	40	25	ES+
TTX	320.1	162.1	0.006	40	38	ES+

References for the MRM Transitions of Hydrophilic Marine Biotoxin

1. Michael J. Boundy,*, Andrew I. Selwood, D. Tim Harwood, Paul S. McNabb, Andrew D. Turner, Barbara Cawthron Journal of Chromatography A, 1387 (2015) 1–12
2. Natural Products From Marine Algae Methods in Molecular Biology

THANK YOU

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