

Waters

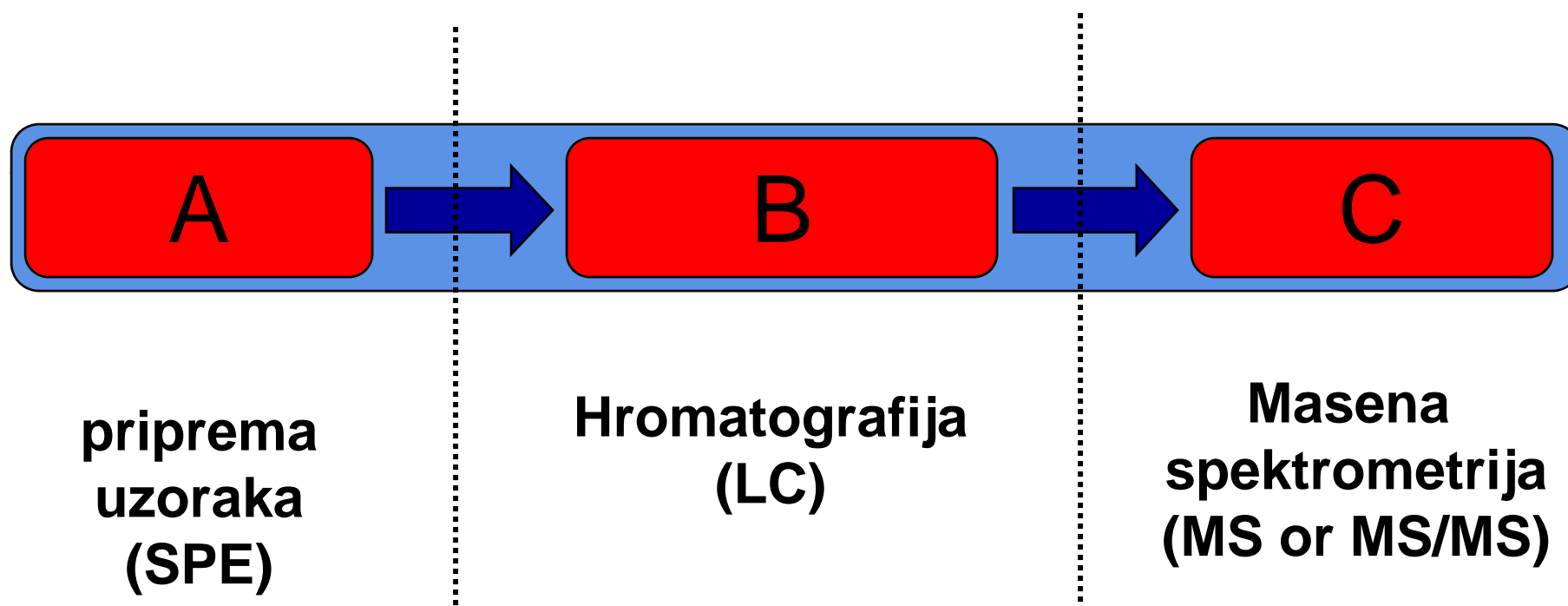
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## WATERS AquaAnalysis System

Online analiza voda

LC/MS-MS





mpen-  
water, solid waste and

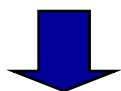
**Priprema  
uzoraka**

**Hromatografija**

**Masena  
Spektrometrija**

**Ne pripremljen uzorak :**

- Voda za pice
- Povrsinske vode
- Otpadne vode
- Sedimenti



**Extracted sample  
For LC/MS/MS**

Ideally, the final sample should be as clean as a non-extracted standard.

**Polarnost:**

Silica- C<sub>18</sub>, C<sub>8</sub>, C<sub>4</sub>, C<sub>2</sub>  
Hybrid- C<sub>18</sub>, C<sub>8</sub>, C<sub>4</sub>, C<sub>2</sub>  
Polymer- C<sub>18</sub>, C<sub>8</sub>, C<sub>4</sub>, C<sub>2</sub>  
Embedded polar group  
Cyano, Phenyl

**Velicina cestice:**

1.8, 2.5, 3.5, 5 or 8 μm

**Unutrasnji dijametar  
kolone :**

4.6, 3.9, 2.1, 1.0,  
0.32 mm and 75 μm

**Duzina kolone:**

150, 100, 50, 30, 20 mm

**Izvor:**

ESI  
APCI  
Nano-ESI

**Maseni  
analizator:**

magnetic sectors  
electric sectors  
time of flight  
quadrupole  
ion trap  
FT-ICR

Moguća rešenja ? ? ? ?

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ACQUITY UPLC™



1525μ



2777 Sample Manager



Acquity SQD



ZQ single quadrupole



LCT Premier ToF



Quattro Premier XE

# Hemija kolona?

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**X-Bridge**  
COLUMNS



**Symmetry**<sup>®</sup>  
Columns



**Acquity**  
Ultra Performance LC™



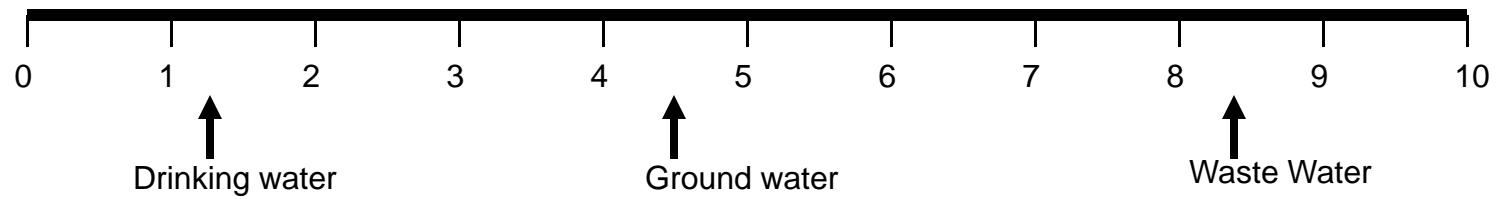
# SPE?

# Waters

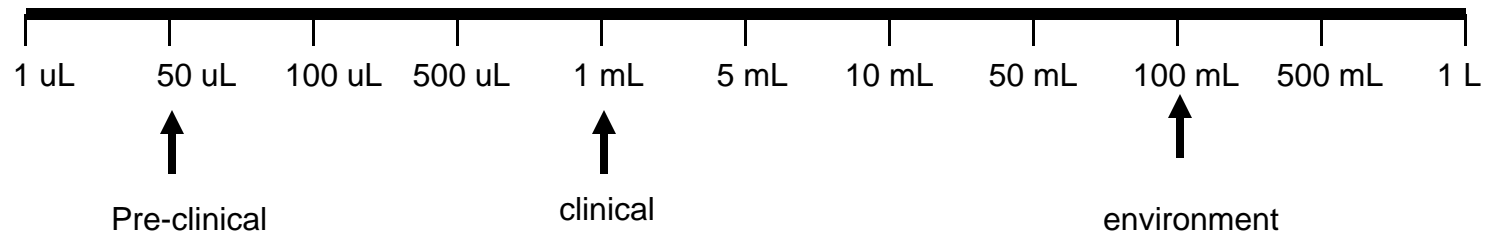
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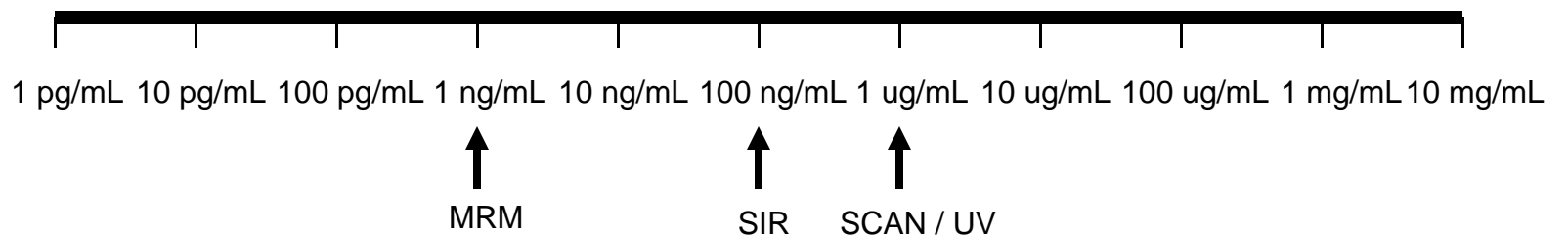
## Kompleksnost matriksa



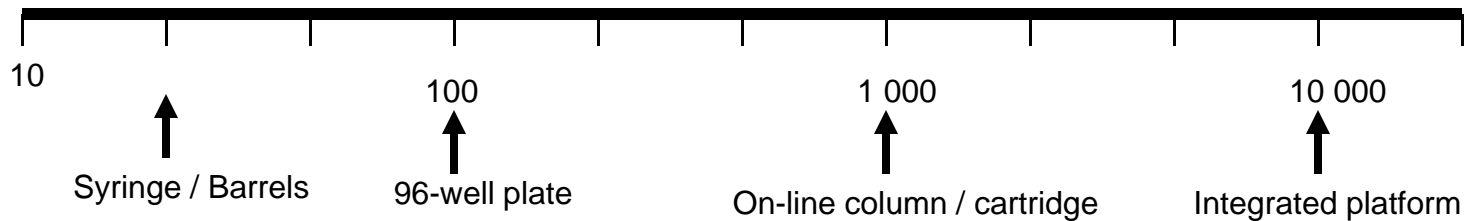
## Raspoloživost zapremine

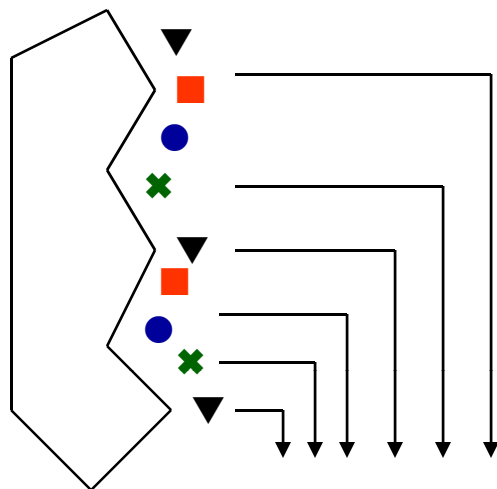


## LOQ

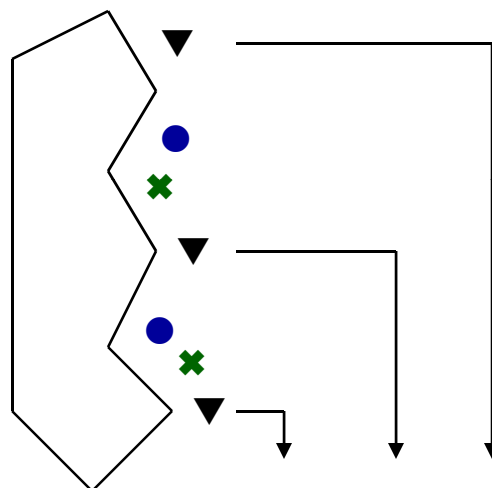


## # uzoraka

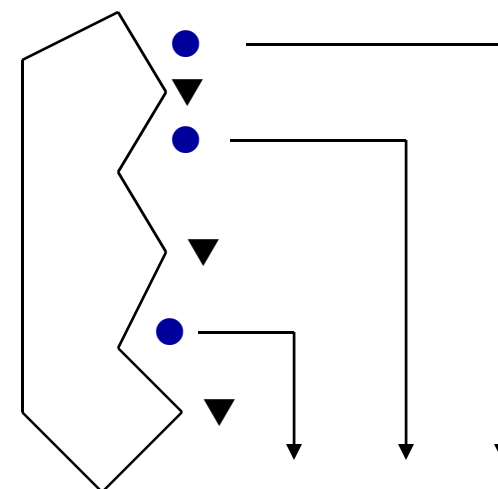




Unselective retention/elution

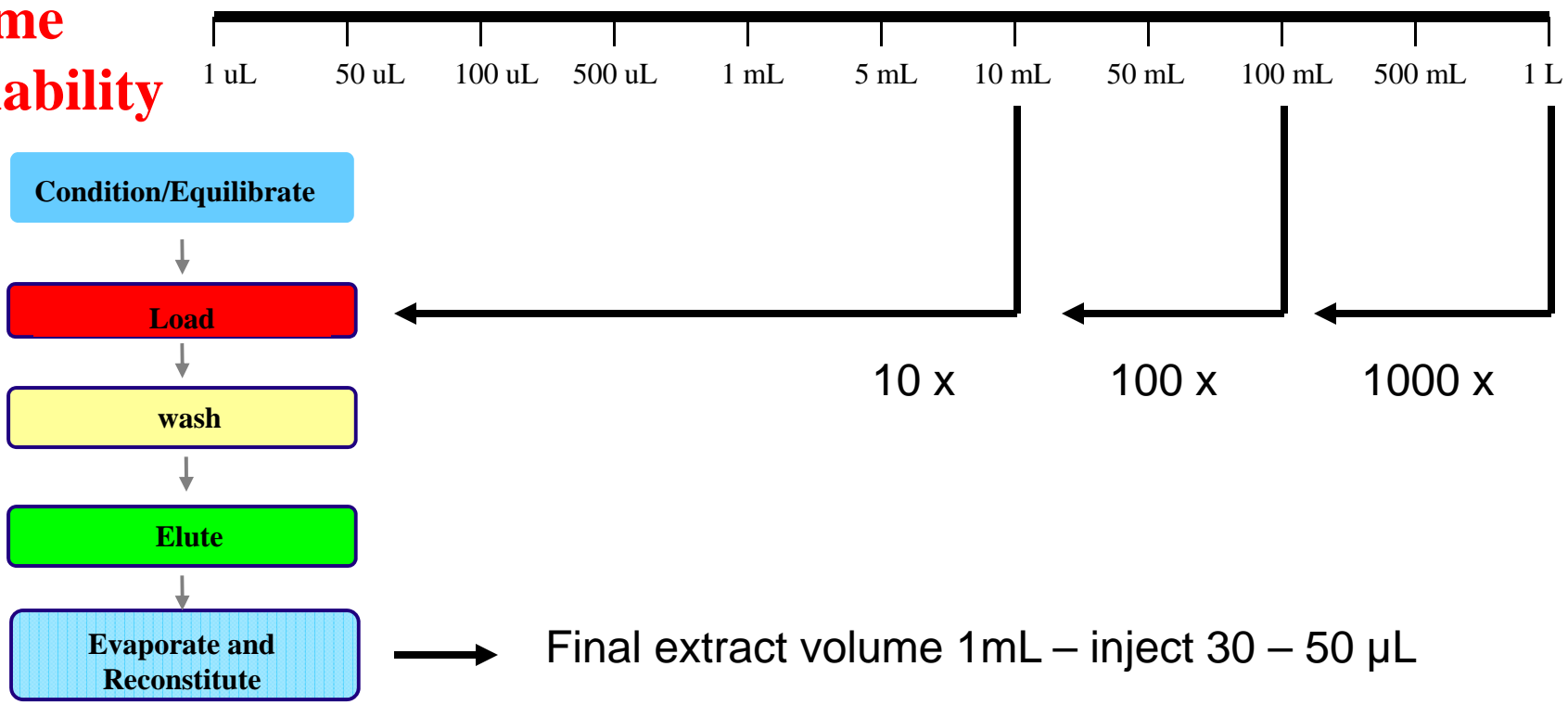


Selective elution

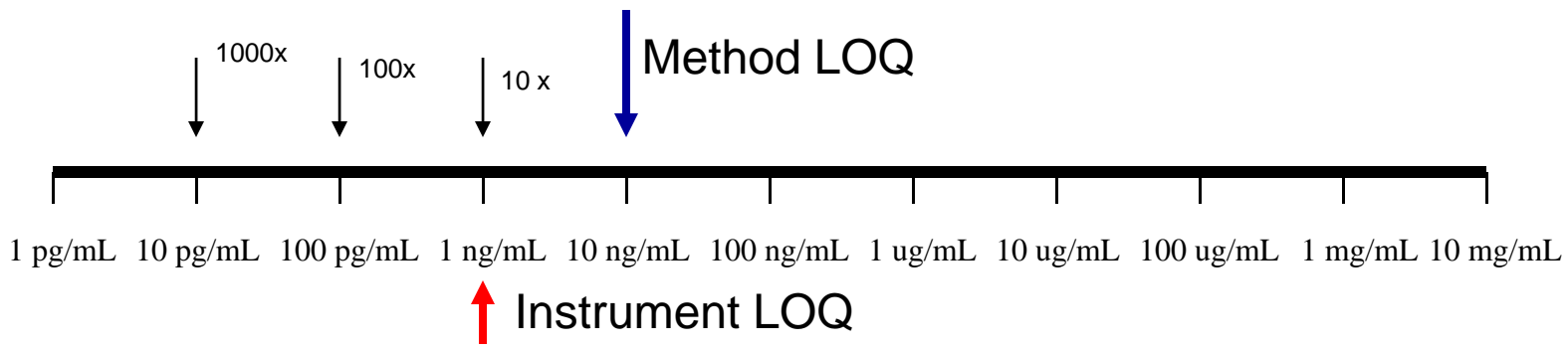


Selection retention/elution

**Volume Availability**



**Target LOQ**



On line/ Off line

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Sample  
Preparation



Chromatography



Mass  
Spectrometry

Off-line SPE



ON-line SPE

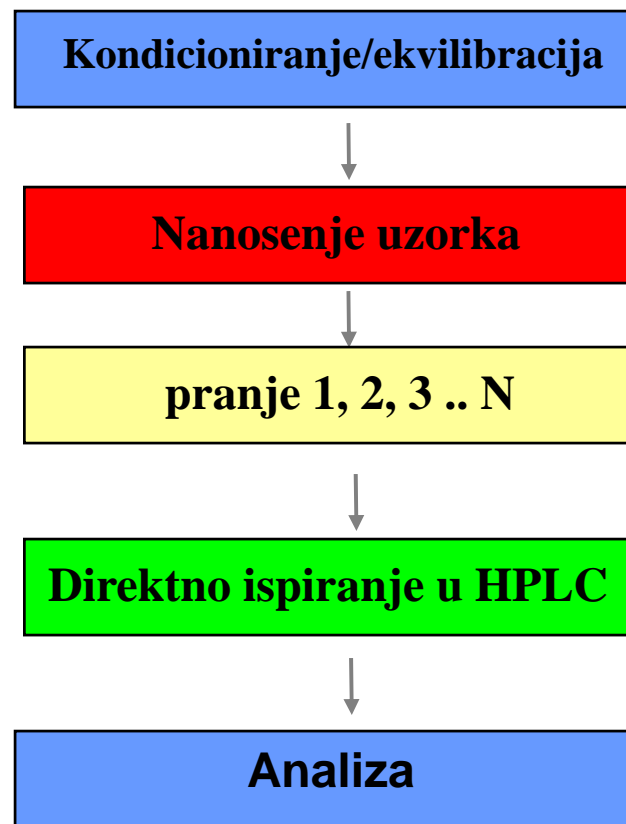


# ON Line SPE Format

ON line analiza je tehnika koja redukuje kolicinu manualnog rada sve do analizabilnog uzorka za to LC/MS/MS.



## Typical ON line SPE Method

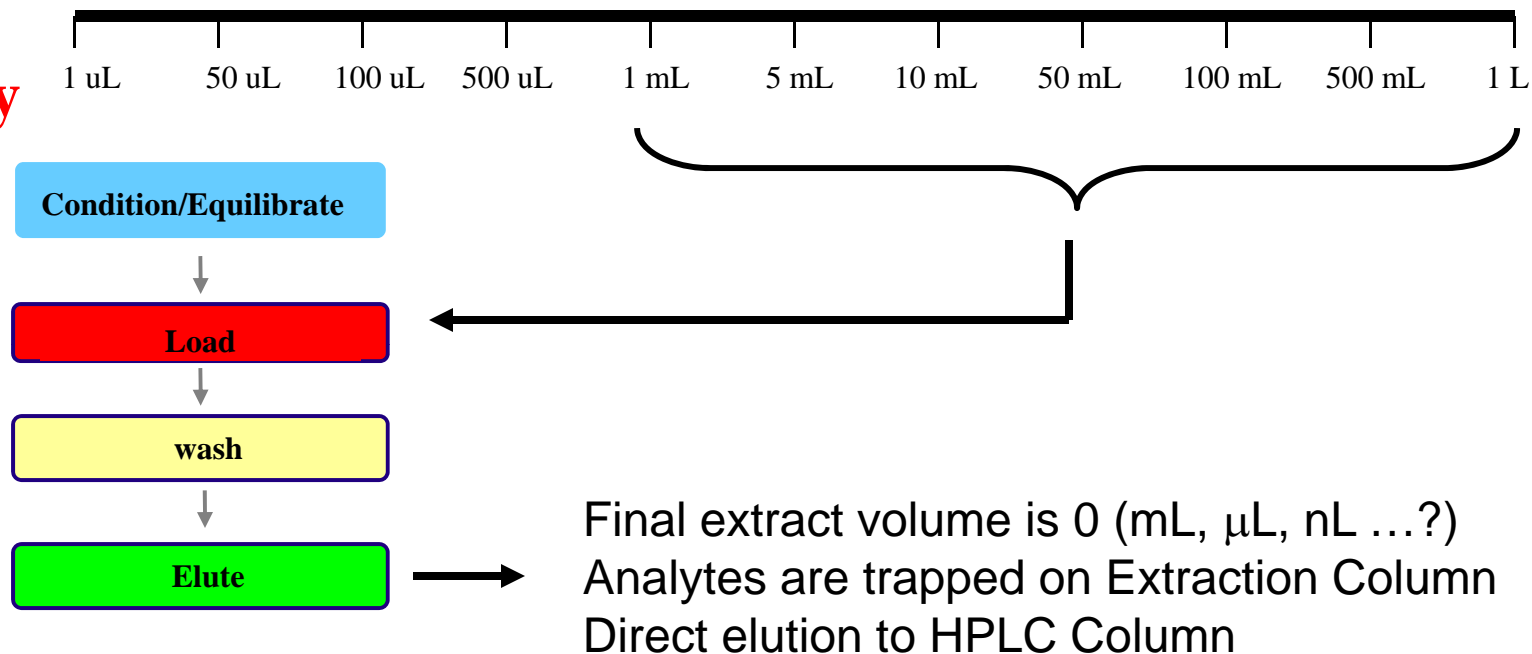


Extraction protocol fully automated

# ON line SPE Volume Equivalency

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## Volume Availability



## Off Line SPE Extraction

## LC/MS Analysis

500 mL (starting volume)  $\longrightarrow$  1 mL final (elution volume)

$\longrightarrow$  30 - 50  $\mu$ L (injection volume)

500:1 enrichment

30  $\mu$ L – 1/33<sup>th</sup> of original volume – 15.1 mL

50  $\mu$ L – 1/20<sup>th</sup> of original volume – 25.0 mL

# OFF-line Vs ON-line Sample Volume

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**1000 mL Container**



**20 mL vial**

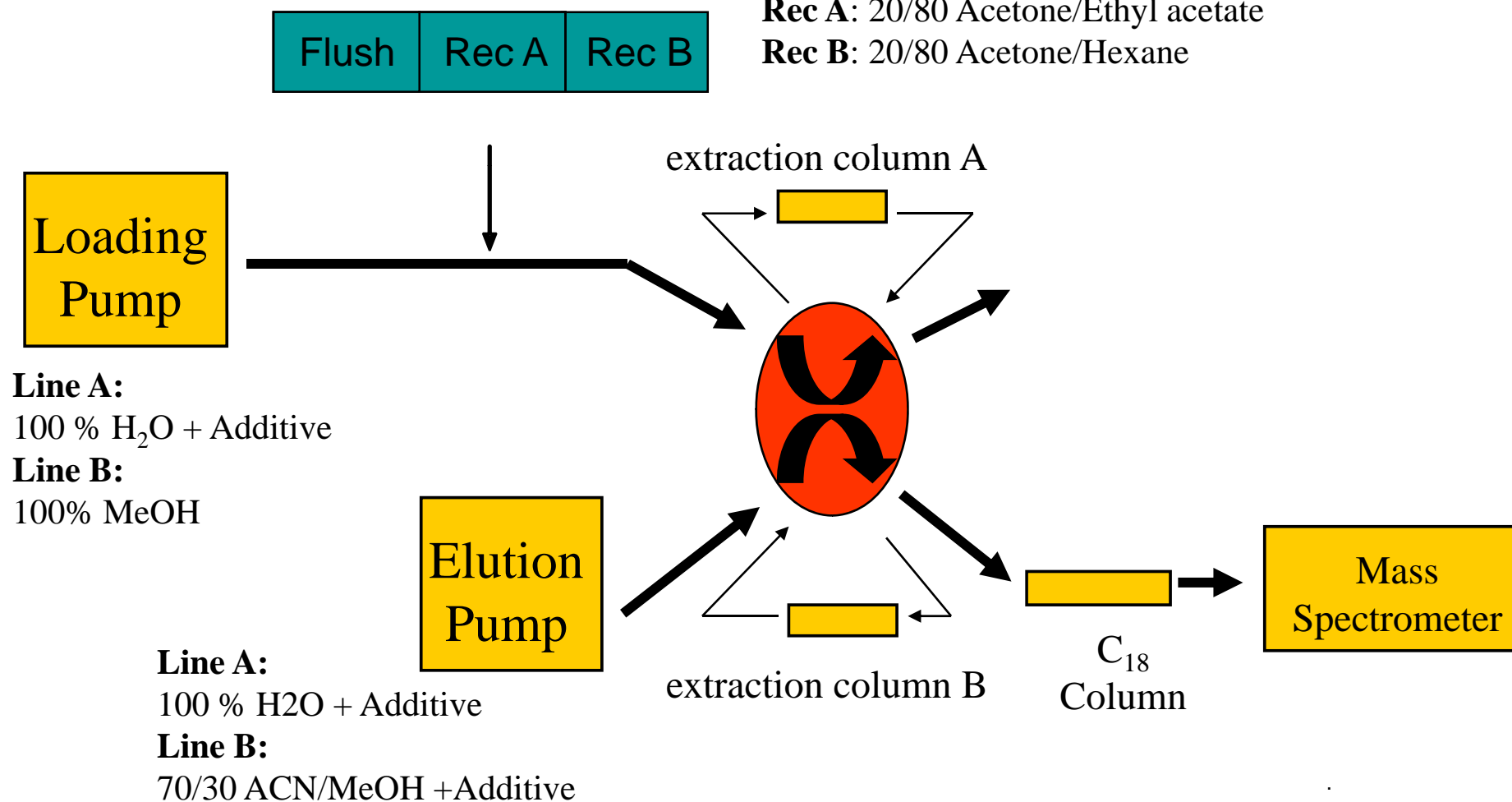
**Autosampler rack**

# Waters AquaAnalysis System (2-1 configuration)

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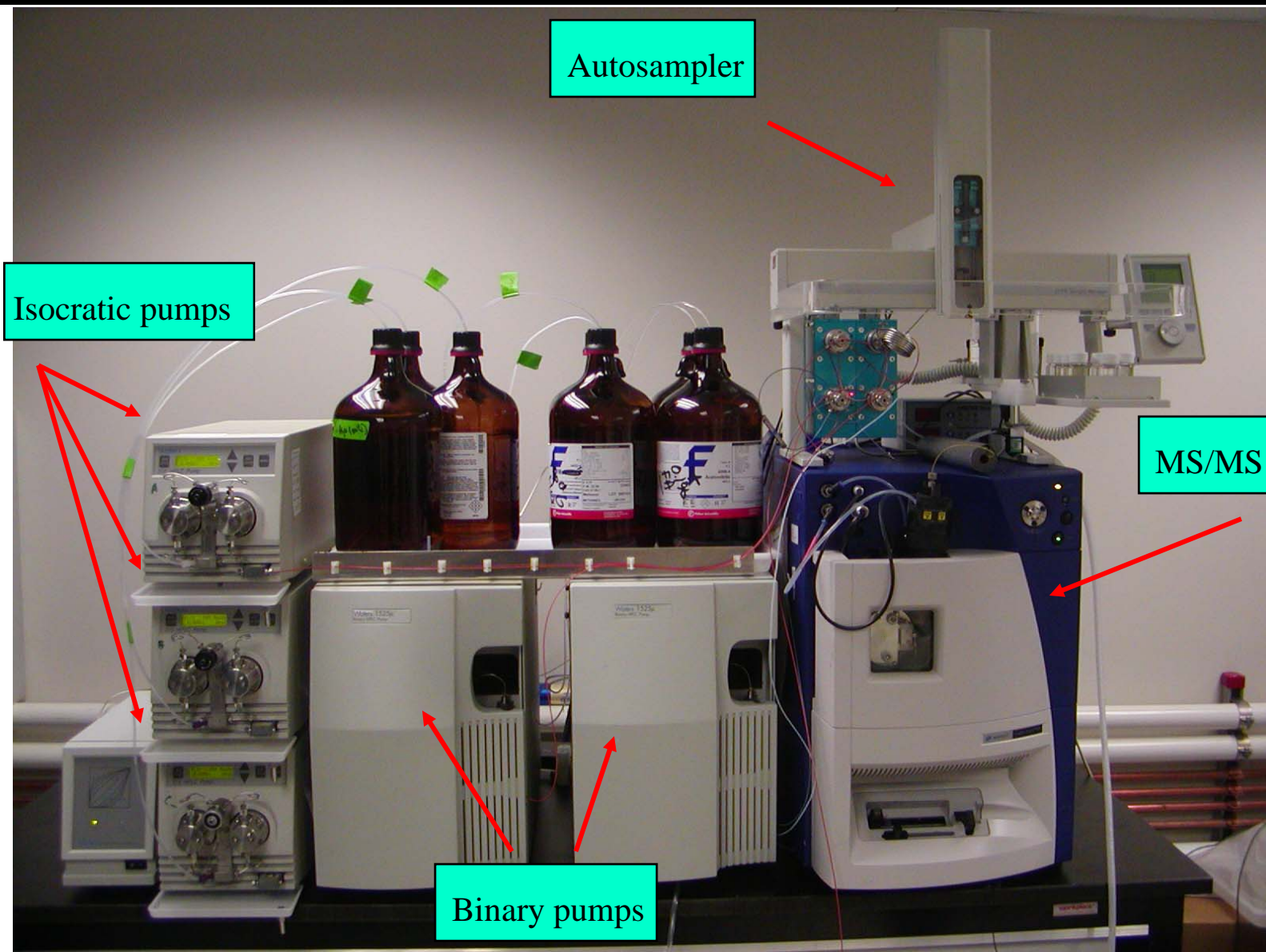
## Parallel<sup>N</sup> SPE (2-1) configuration

**Flush:** 50/50 Acetonitrile/Acetone  
**Rec A:** 20/80 Acetone/Ethyl acetate  
**Rec B:** 20/80 Acetone/Hexane



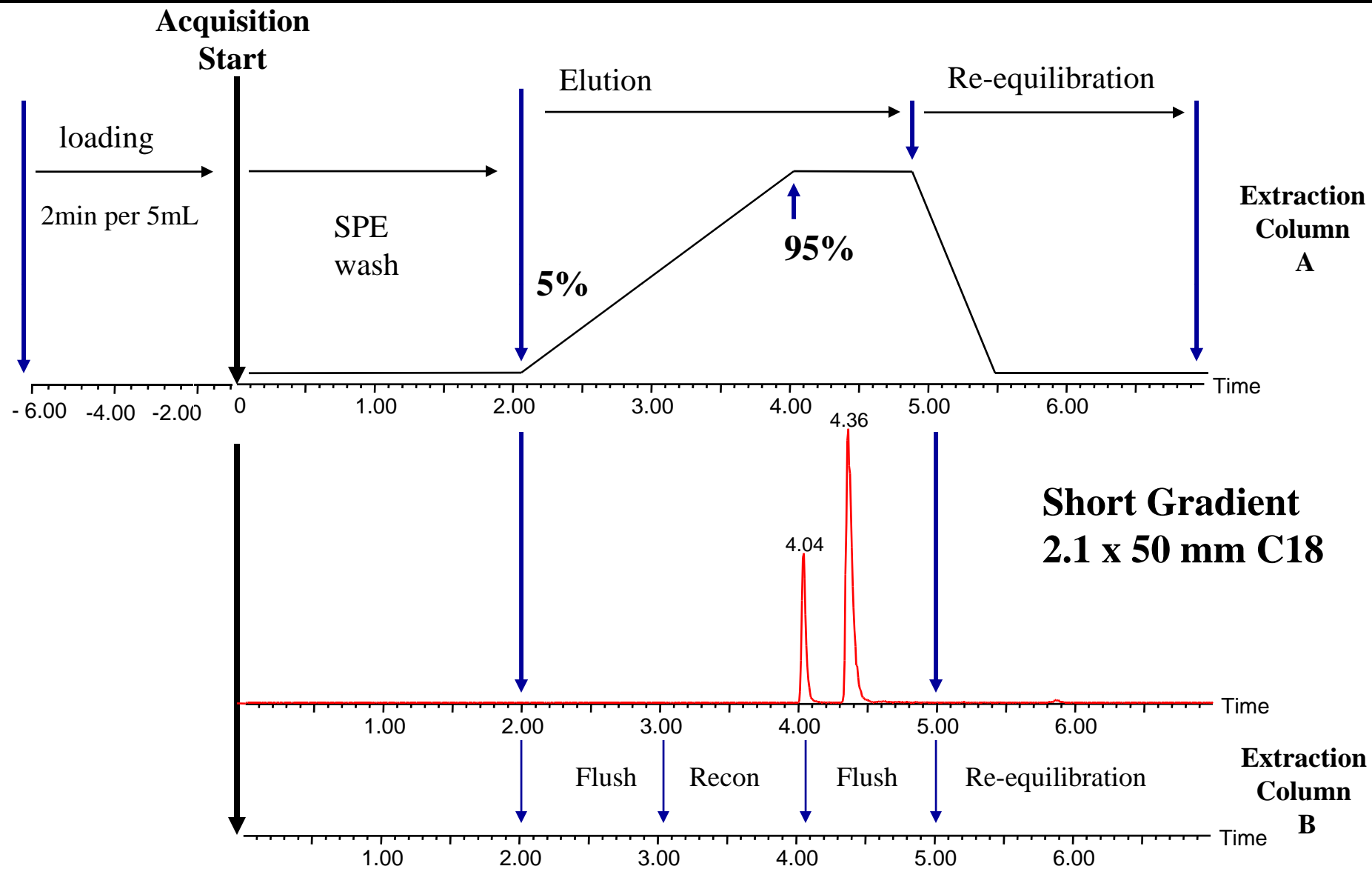
# Waters AquaAnalysis (2-1 configuration)

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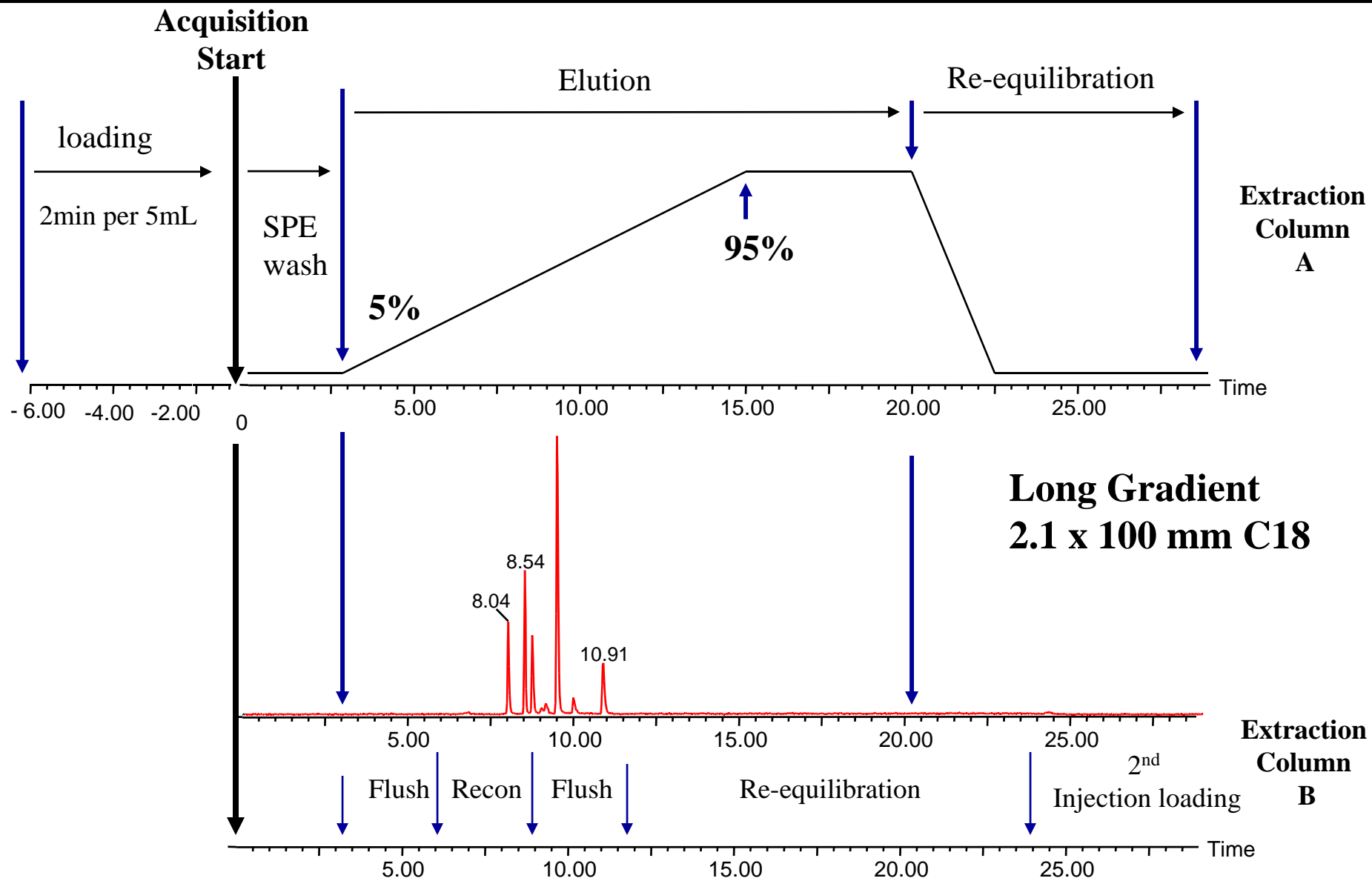
# Waters AquaAnalysis System (2-1 configuration) Sequential and Parallel Events

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# AquaAnalysis System (2-1 configuration) Sequential and Parallel Events

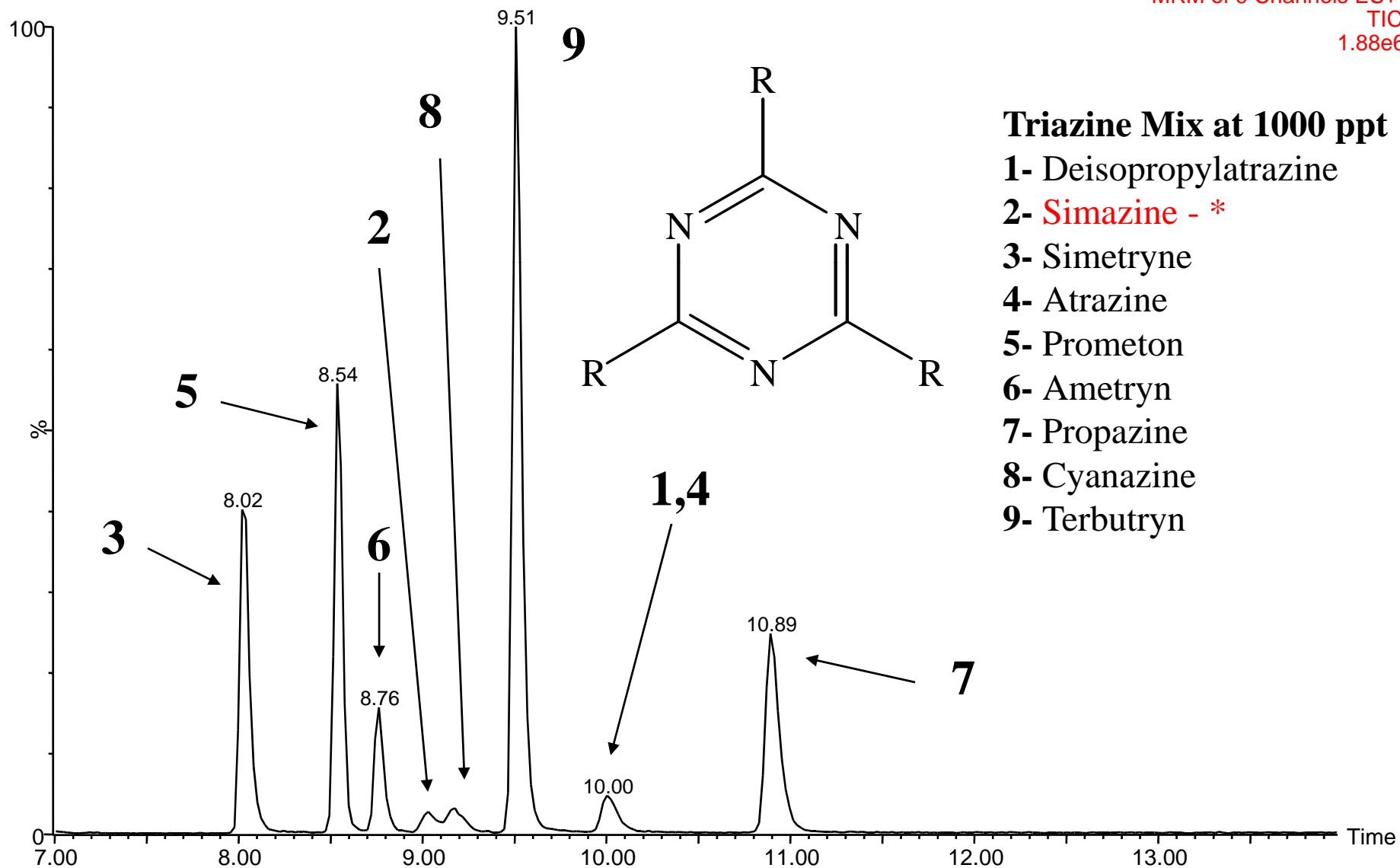
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# Triazines Mix 1 mL Loading Volume

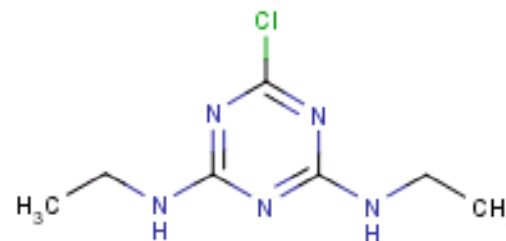
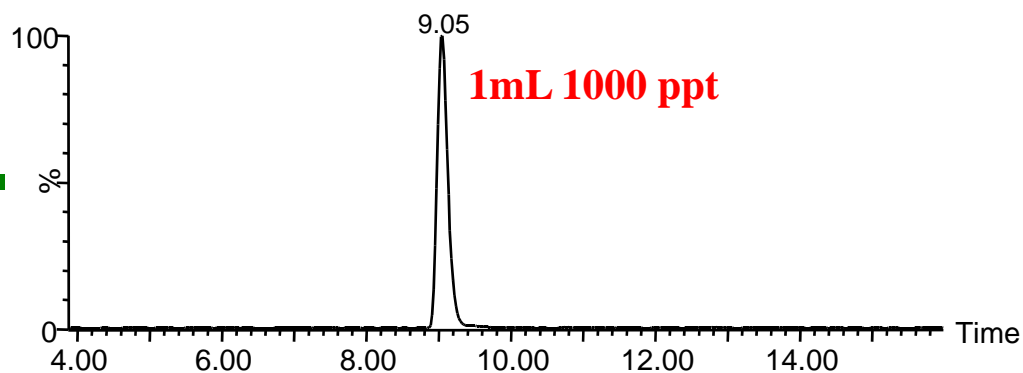
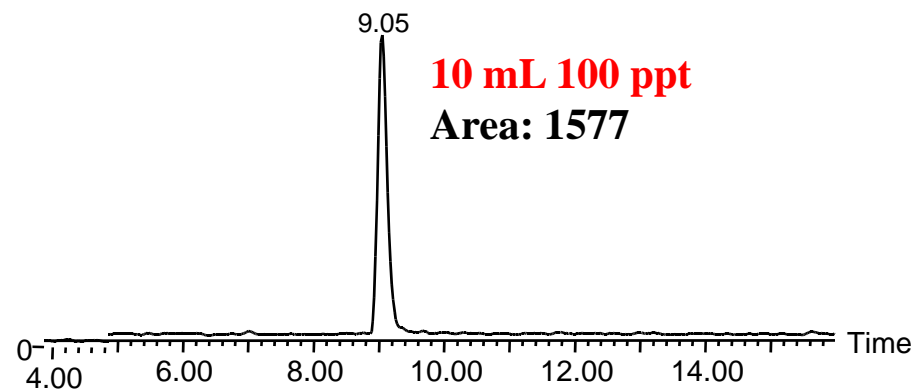
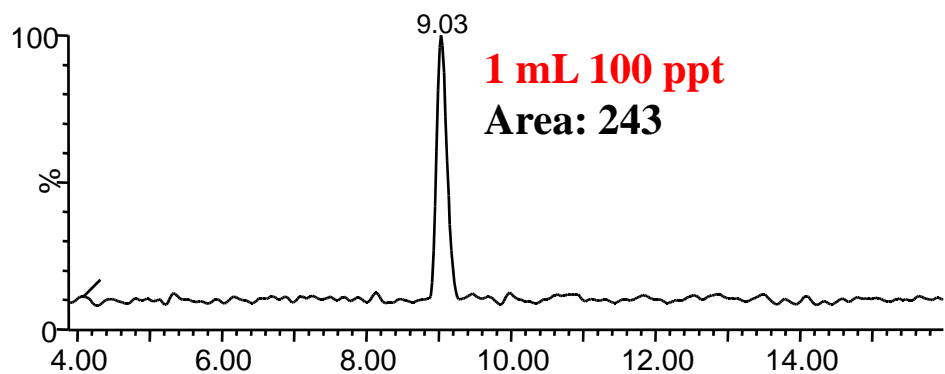
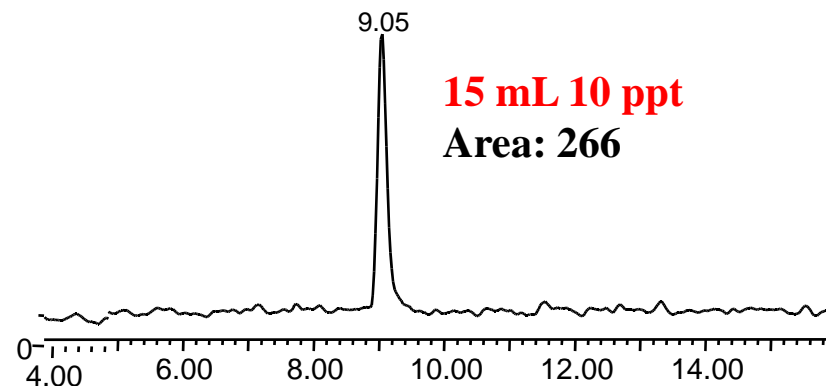
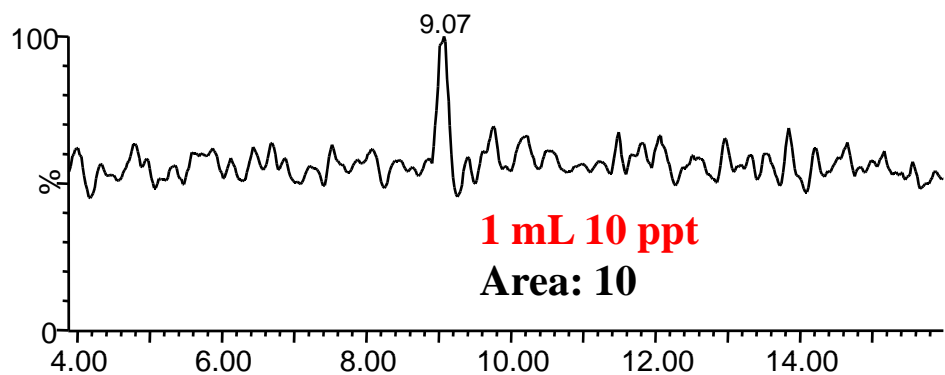
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MRM of 9 Channels ES+  
TIC  
1.88e6



# Simazine Loading Volume

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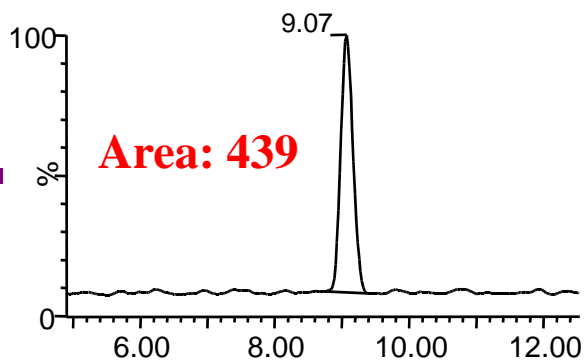
- Average of 10 injections
- CV > 10 %

# Loading Conditions Low, Neutral and High pH

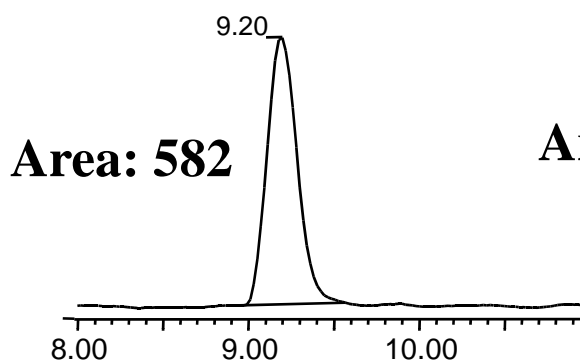
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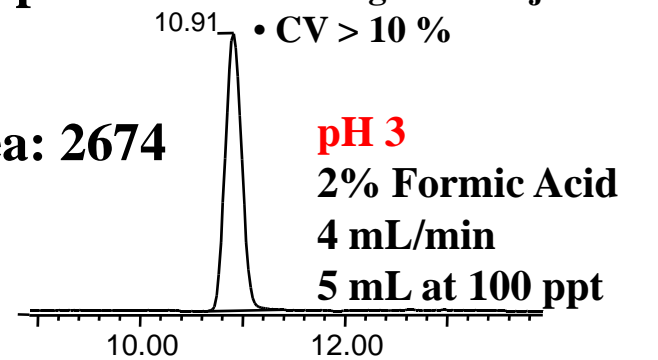
### Simazine



### Cyanazine

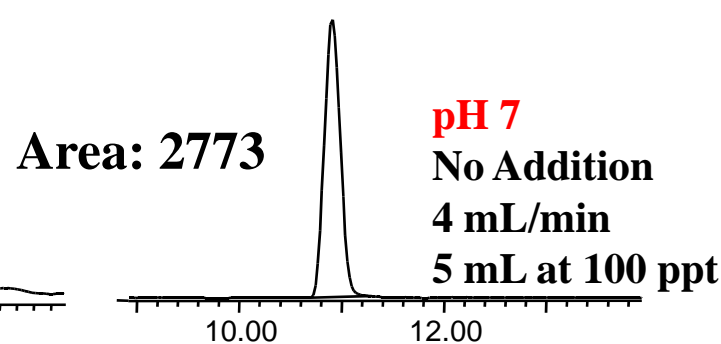
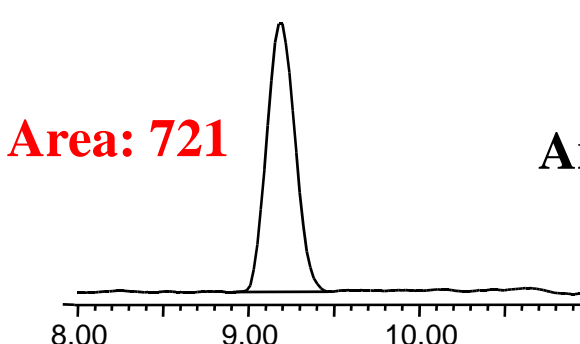
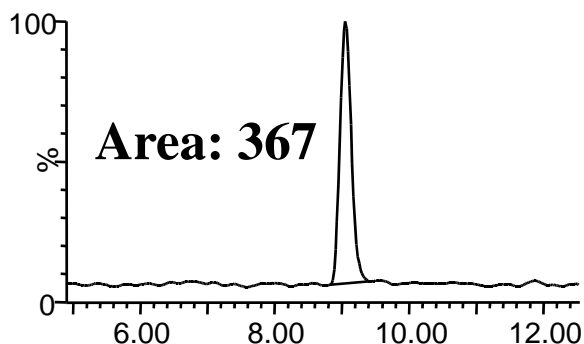


### Propazine

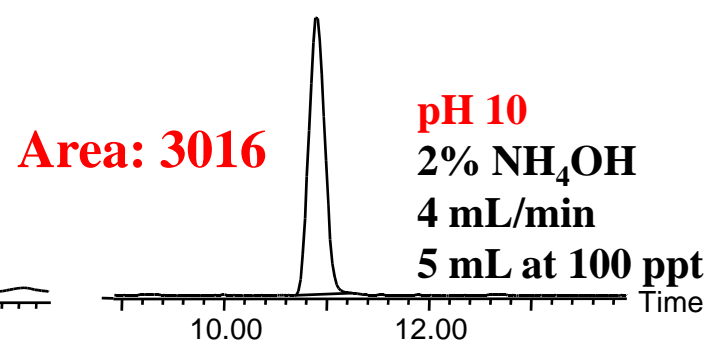
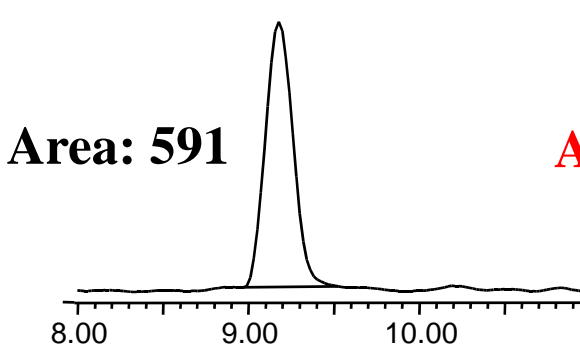
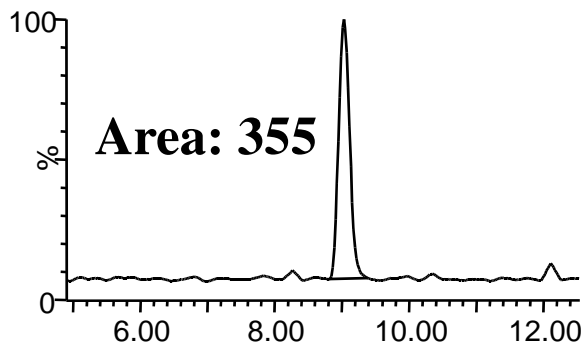


- Average of 10 injections
- CV > 10 %

**pH 3**  
2% Formic Acid  
4 mL/min  
5 mL at 100 ppt



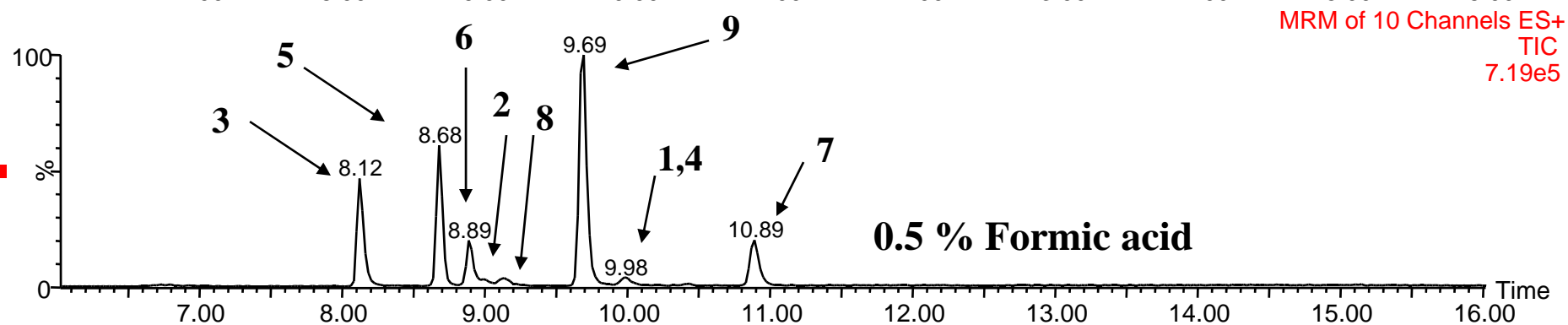
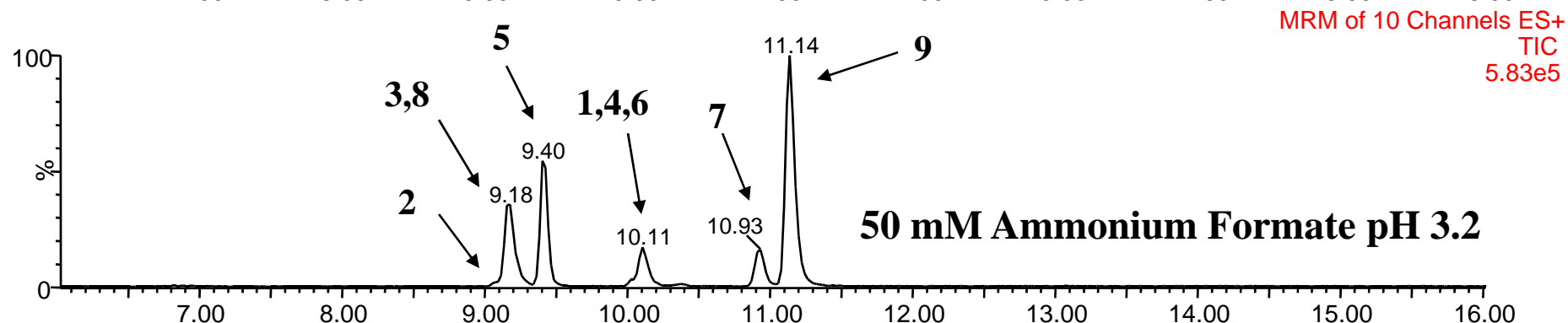
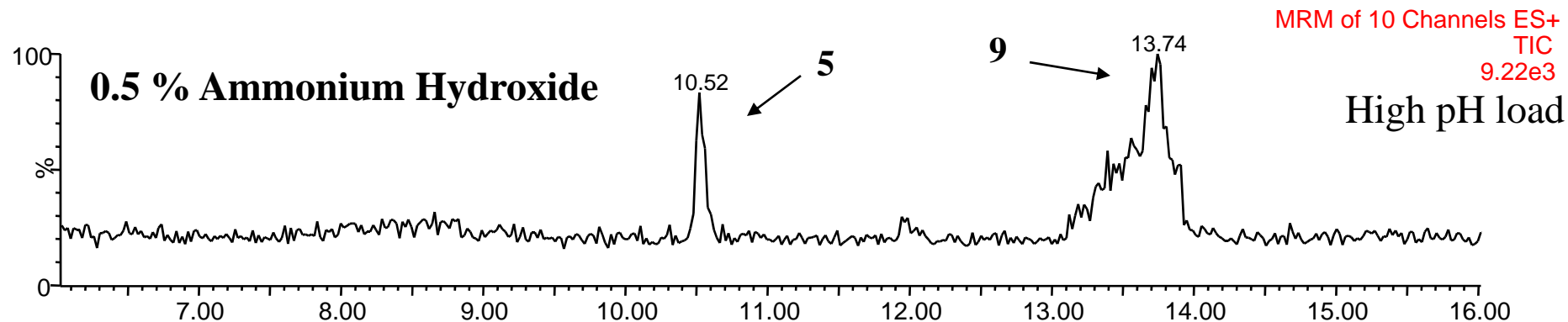
**pH 7**  
No Addition  
4 mL/min  
5 mL at 100 ppt



**pH 10**  
2% NH<sub>4</sub>OH  
4 mL/min  
5 mL at 100 ppt

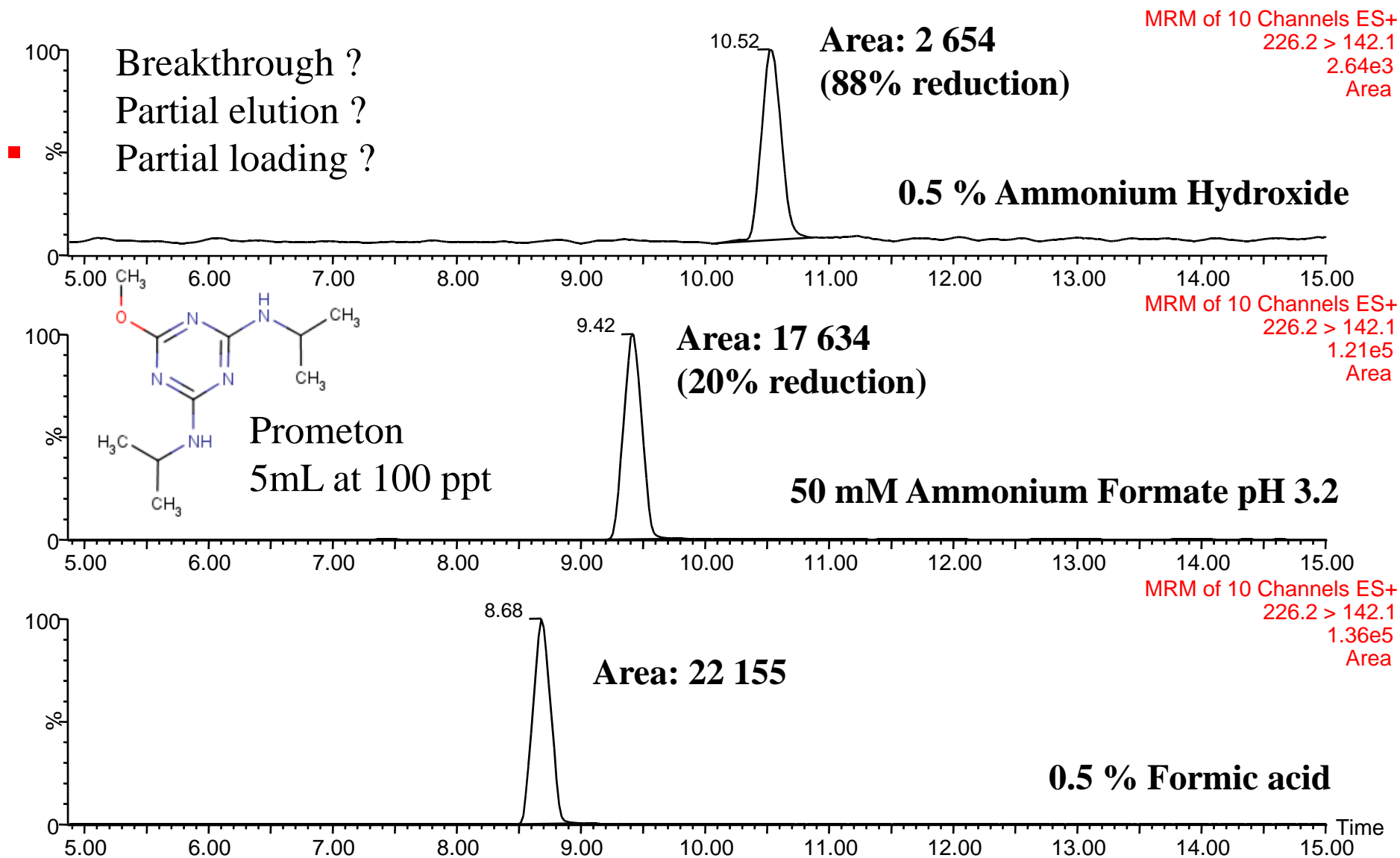
# Eluting Conditions Low and High pH

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# Eluting Conditions Low and High pH

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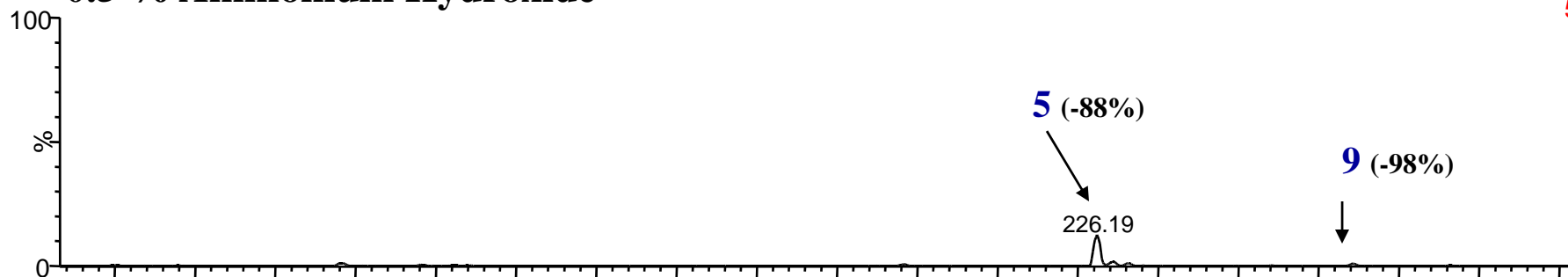


# Infusion Triazines Mix at 1 ppm : Low and High pH

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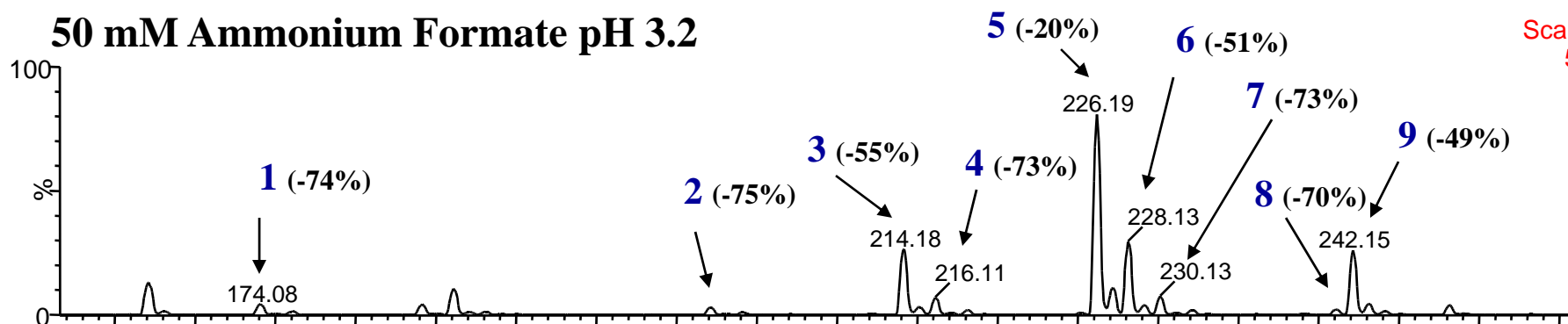
Scan ES+  
5.28e9

## 0.5 % Ammonium Hydroxide



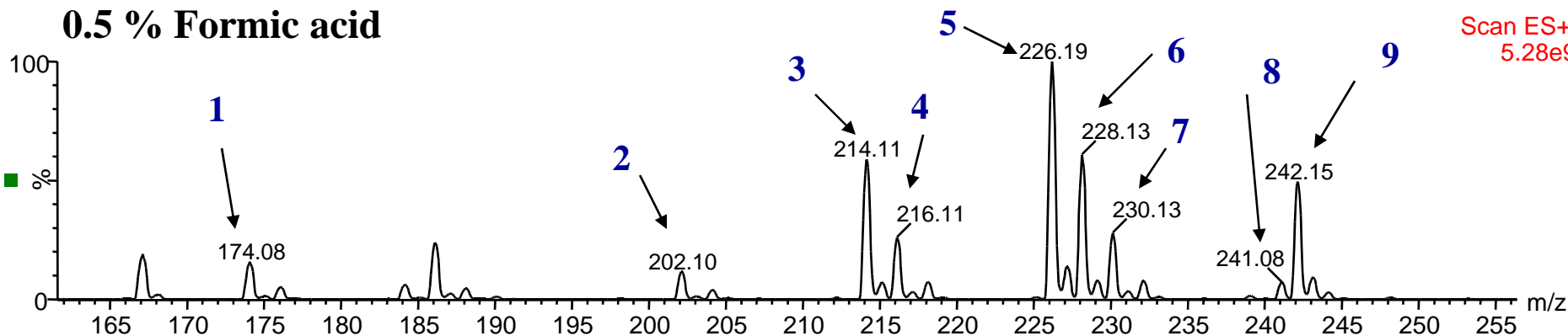
Scan ES+  
5.28e9

## 50 mM Ammonium Formate pH 3.2



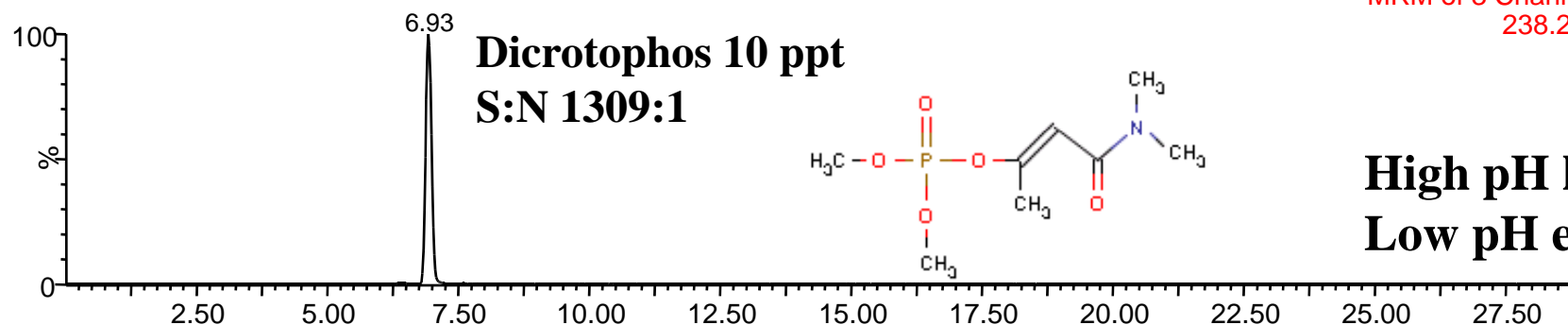
Scan ES+  
5.28e9

## 0.5 % Formic acid



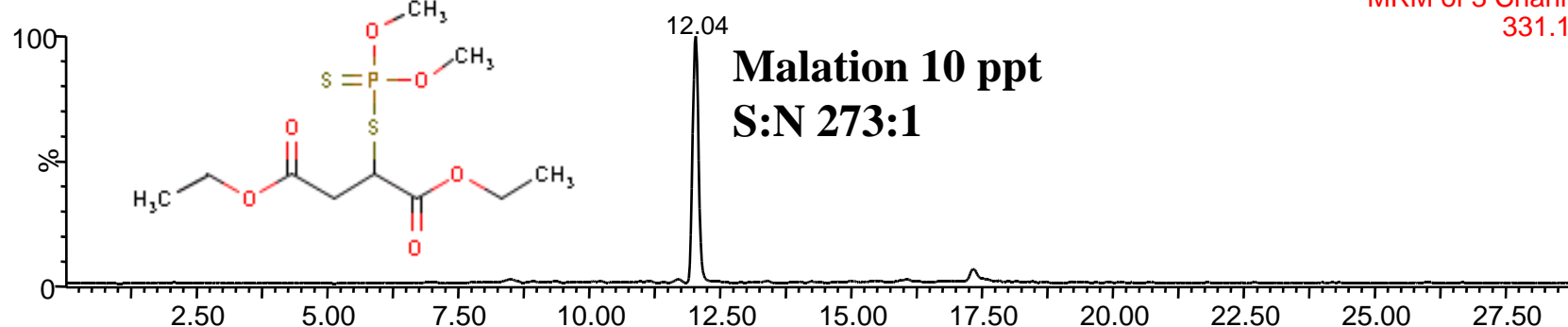
# Organophosphorous 15 mL Water Sample 10 ppt

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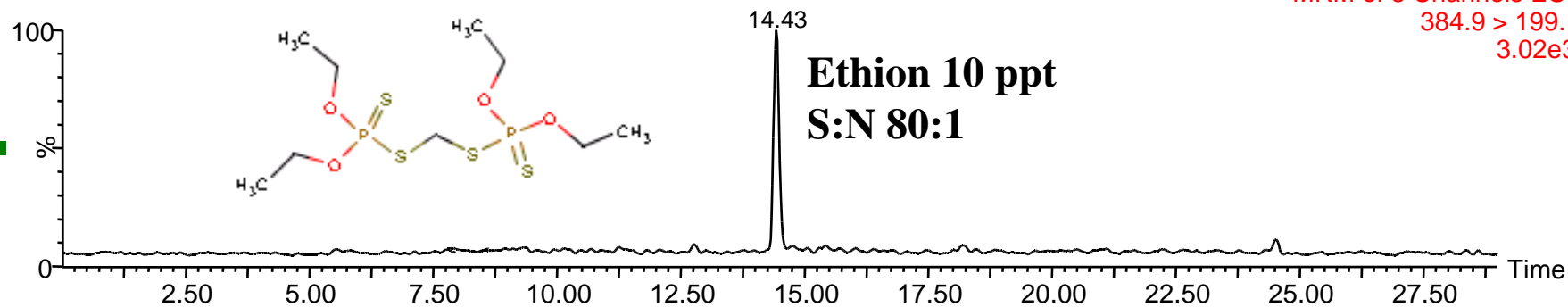


MRM of 3 Channels ES+  
238.2 > 111.8  
7.55e4

**High pH load**  
**Low pH elution**



MRM of 3 Channels ES+  
331.1 > 126.9  
1.10e4

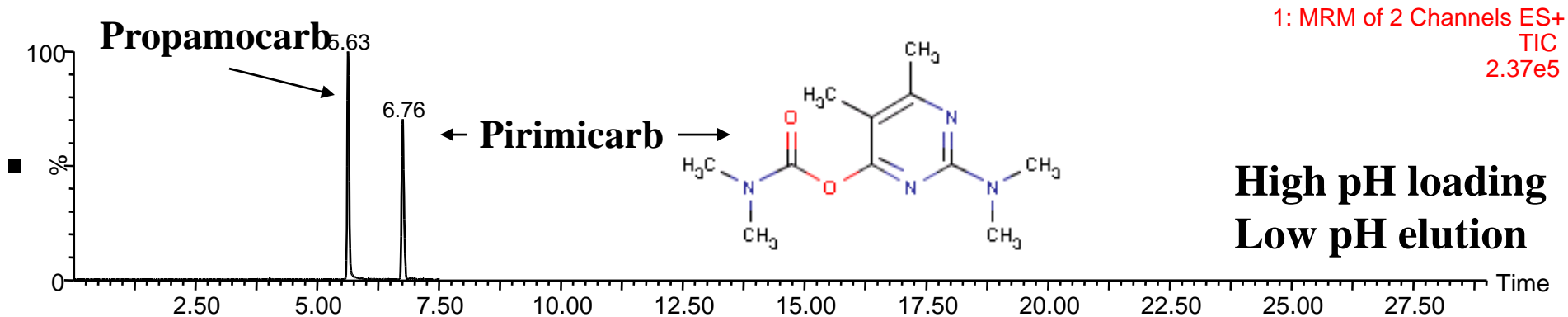
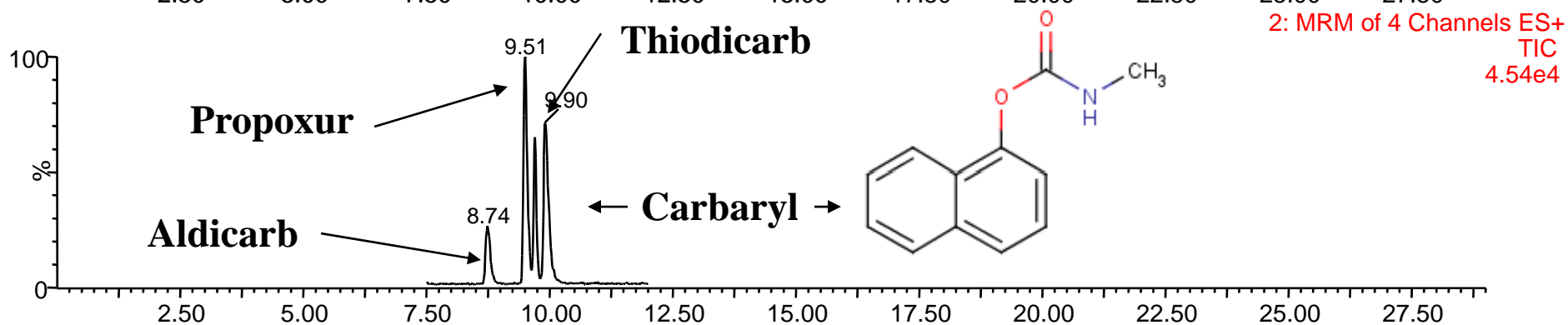
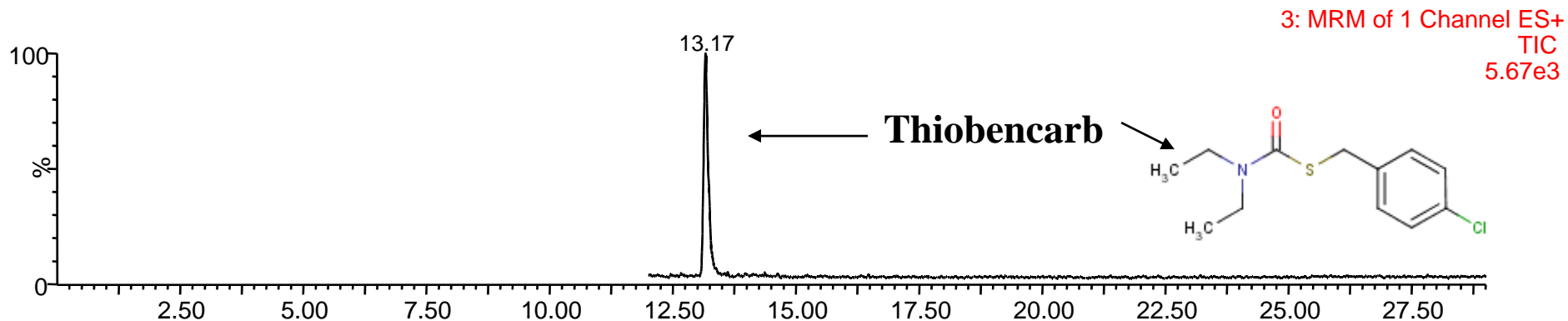


MRM of 3 Channels ES+  
384.9 > 199.1  
3.02e3

# Carbamates

## 15 mL Water Sample 10 ppt

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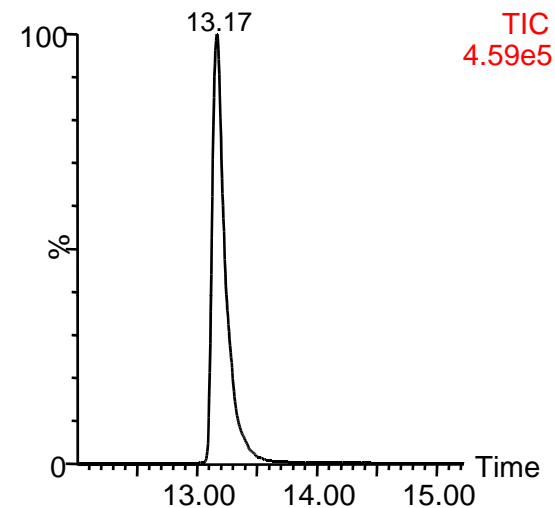
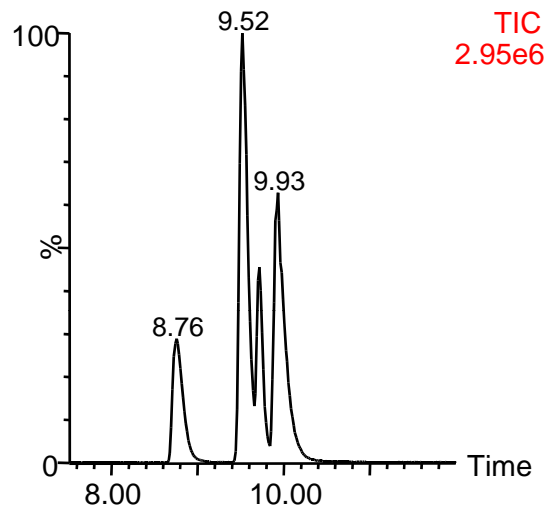
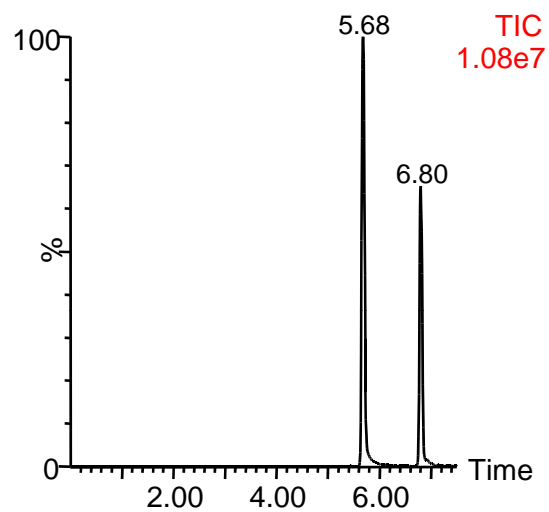


**High pH loading**  
**Low pH elution**

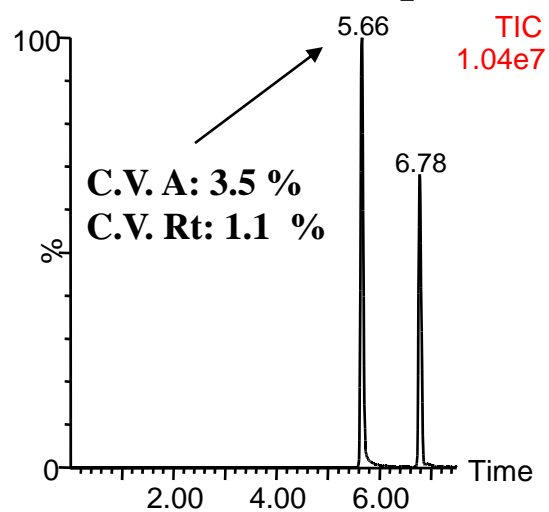
# Robustness 1 mL volume at 1000 ppt

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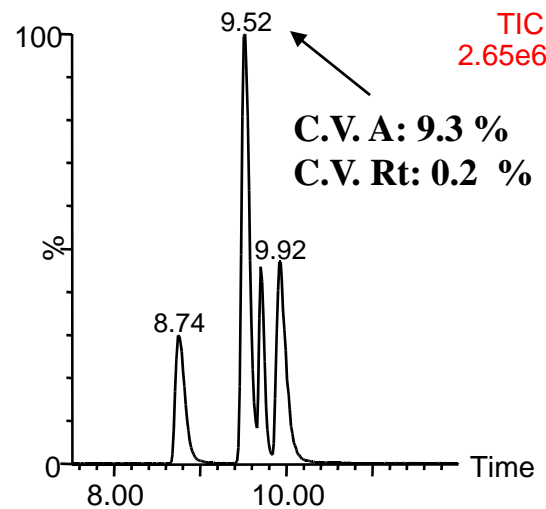
## Injection # 1



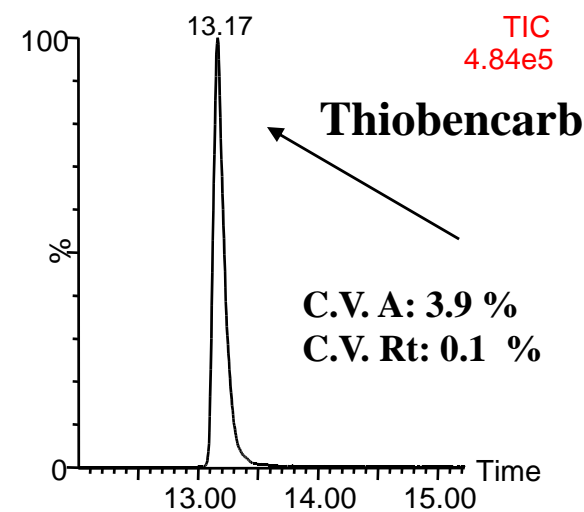
## Injection # 50 Propamocarb



## Propoxur

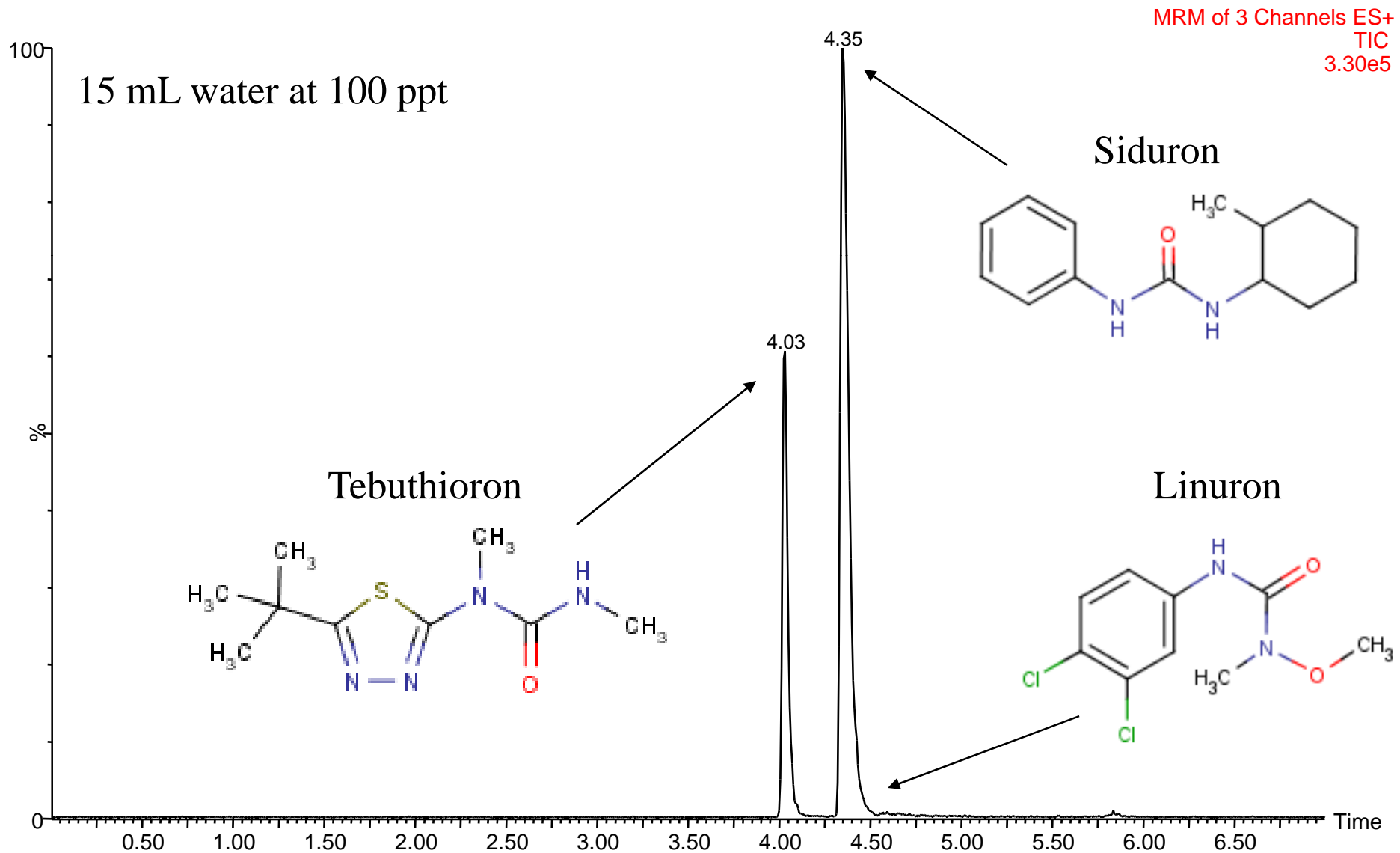


## Thiobencarb



# Extraction Column Lifetime Organo-nitrogen

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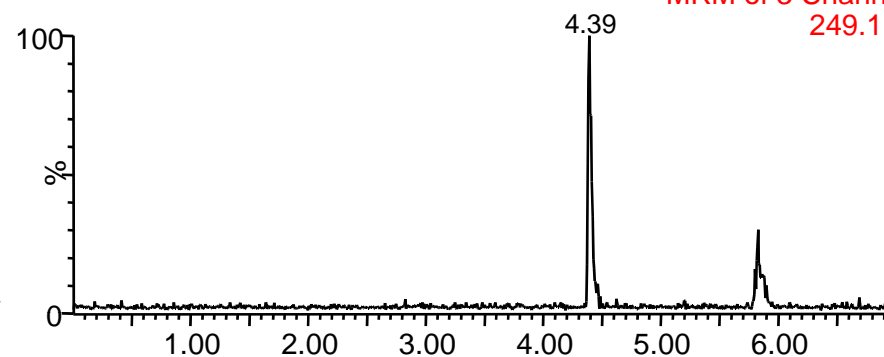
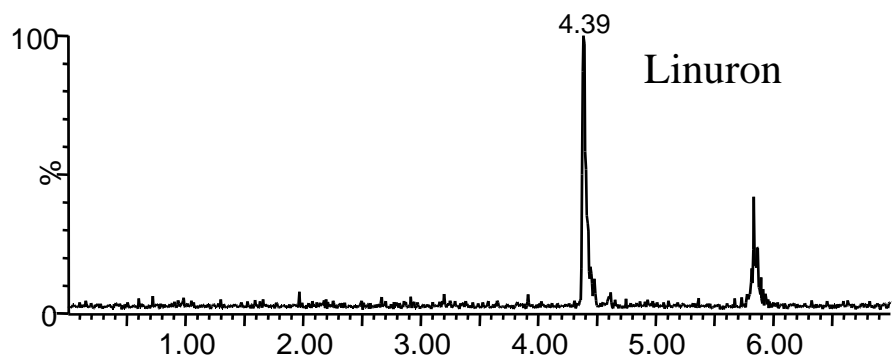


# Column Lifetime Organo-nitrogen

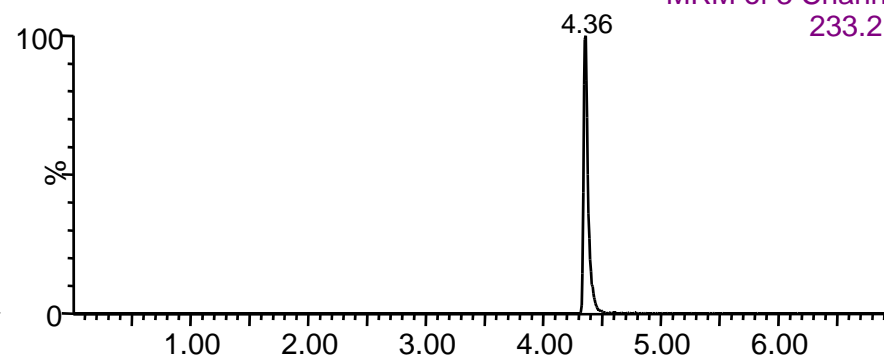
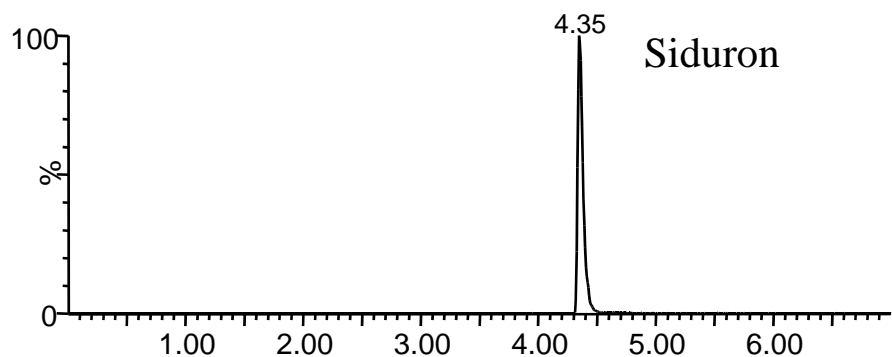
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1<sup>th</sup> injection

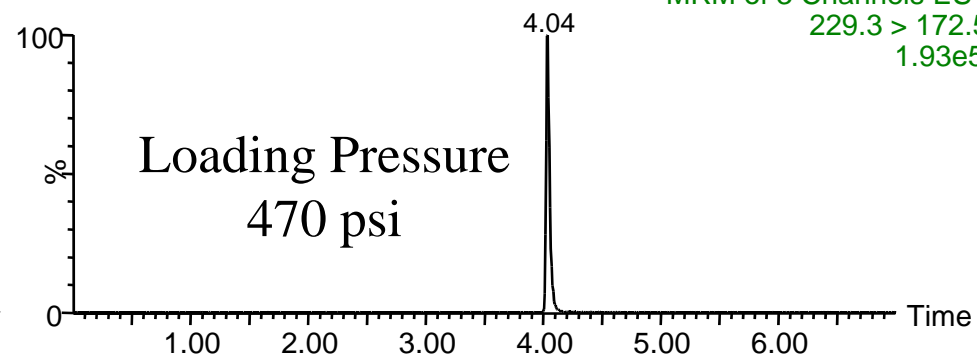
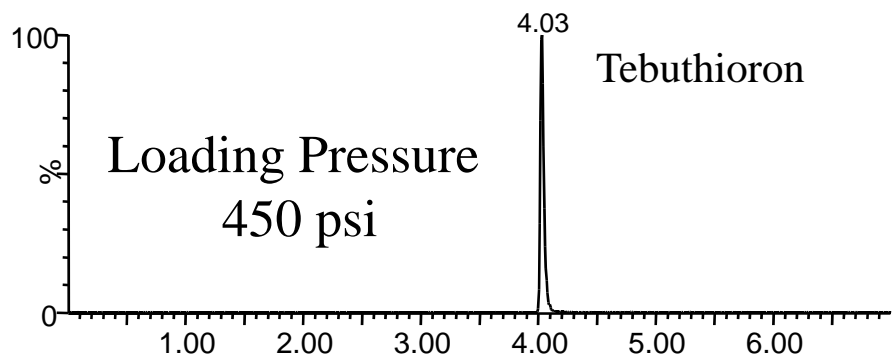
500<sup>th</sup> injection



MRM of 3 Channels ES+  
249.1 > 160.3  
8.35e3



MRM of 3 Channels ES+  
233.2 > 137.4  
3.91e5



MRM of 3 Channels ES+  
229.3 > 172.5  
1.93e5

Potpuno automatizovan sistem

Limiti detekcije ng/mL LOQ's

Minimalizovana priprema

Redukovan manualni rad

Kompatibilnost SPE i hromatografskih kolona

Reproduktivnost i robusnost