



# From Trend to Discovery: Temporal Analysis of Contaminants in Watersheds Using High Resolution Mass Spectrometry

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- Temporal monitoring
  - What is it?
  - How has it been used previously?
  - Rhine River research
- High resolution mass spectrometry for non-targeted analysis
- Our own monitoring study
  - Watershed
  - Sample collection
  - HRMS Analysis
  - Data Analysis
    - enviMass
    - ChemSpider
  - Trends and compounds discovered

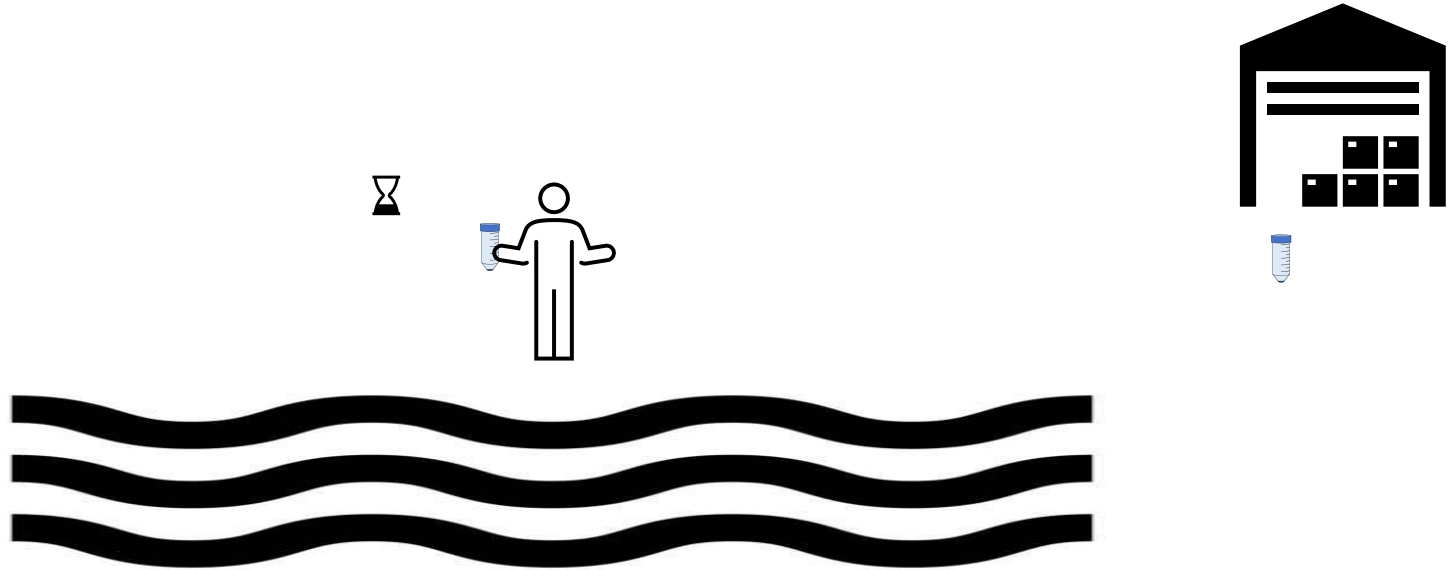
# Spatio-Temporal Monitoring



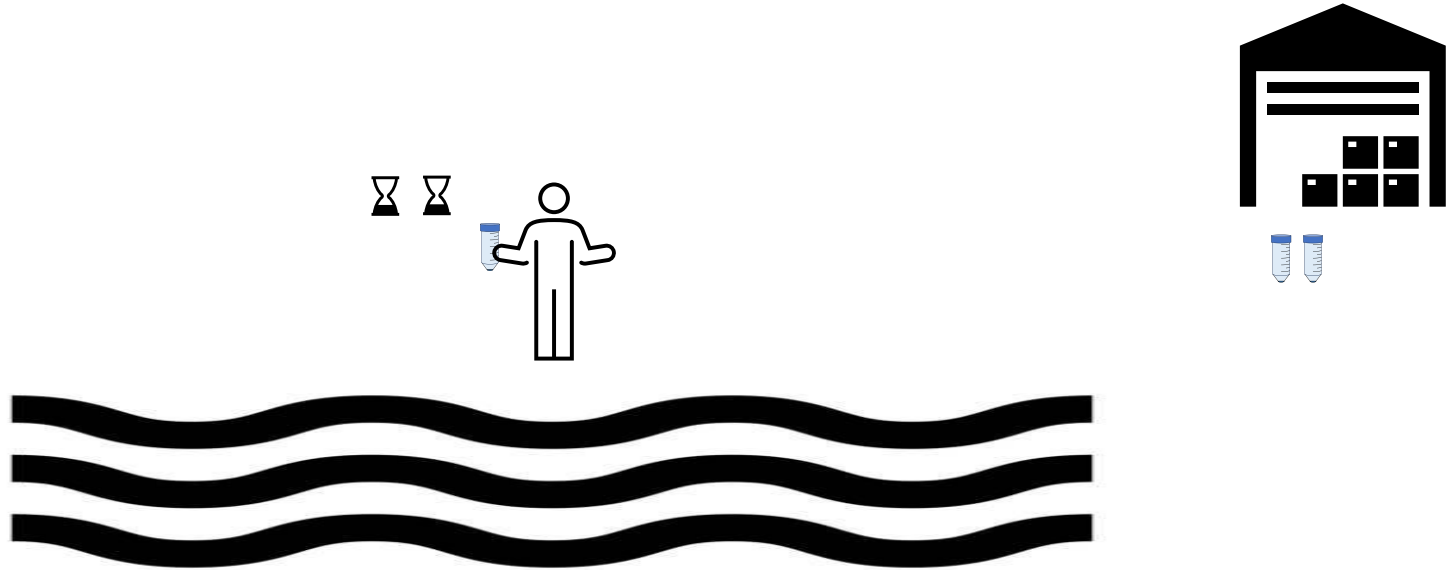
# Spatio-Temporal Monitoring



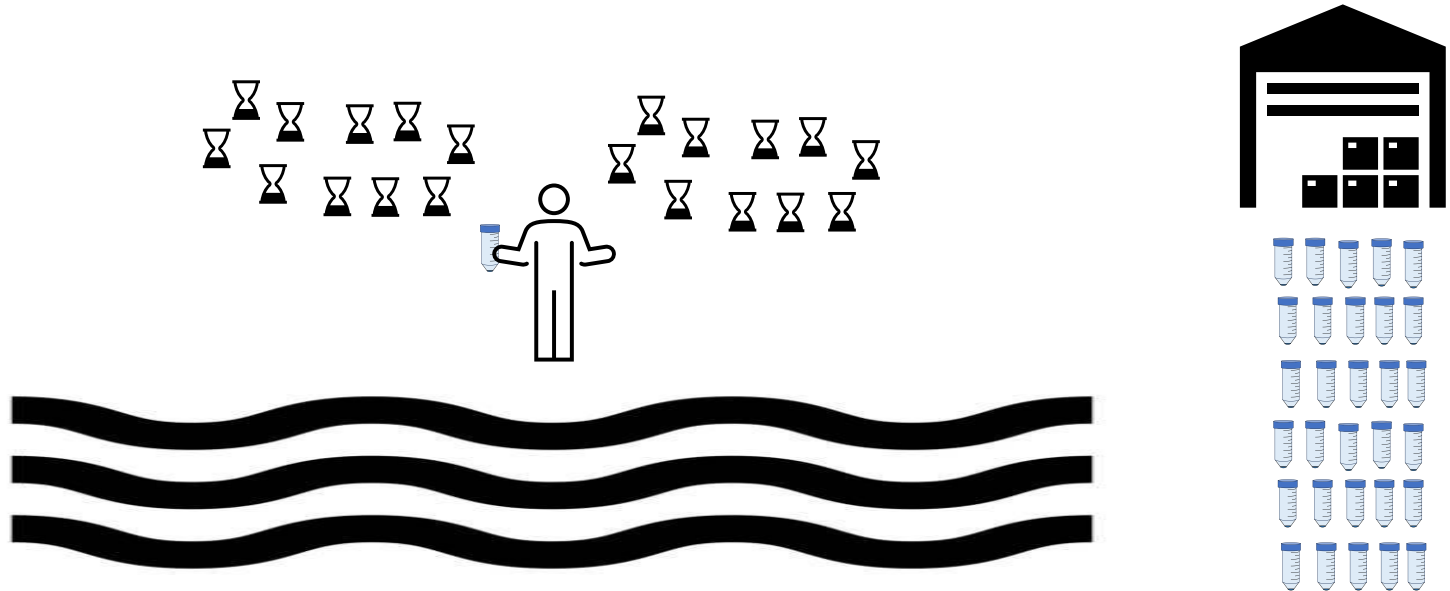
# Spatio-Temporal Monitoring



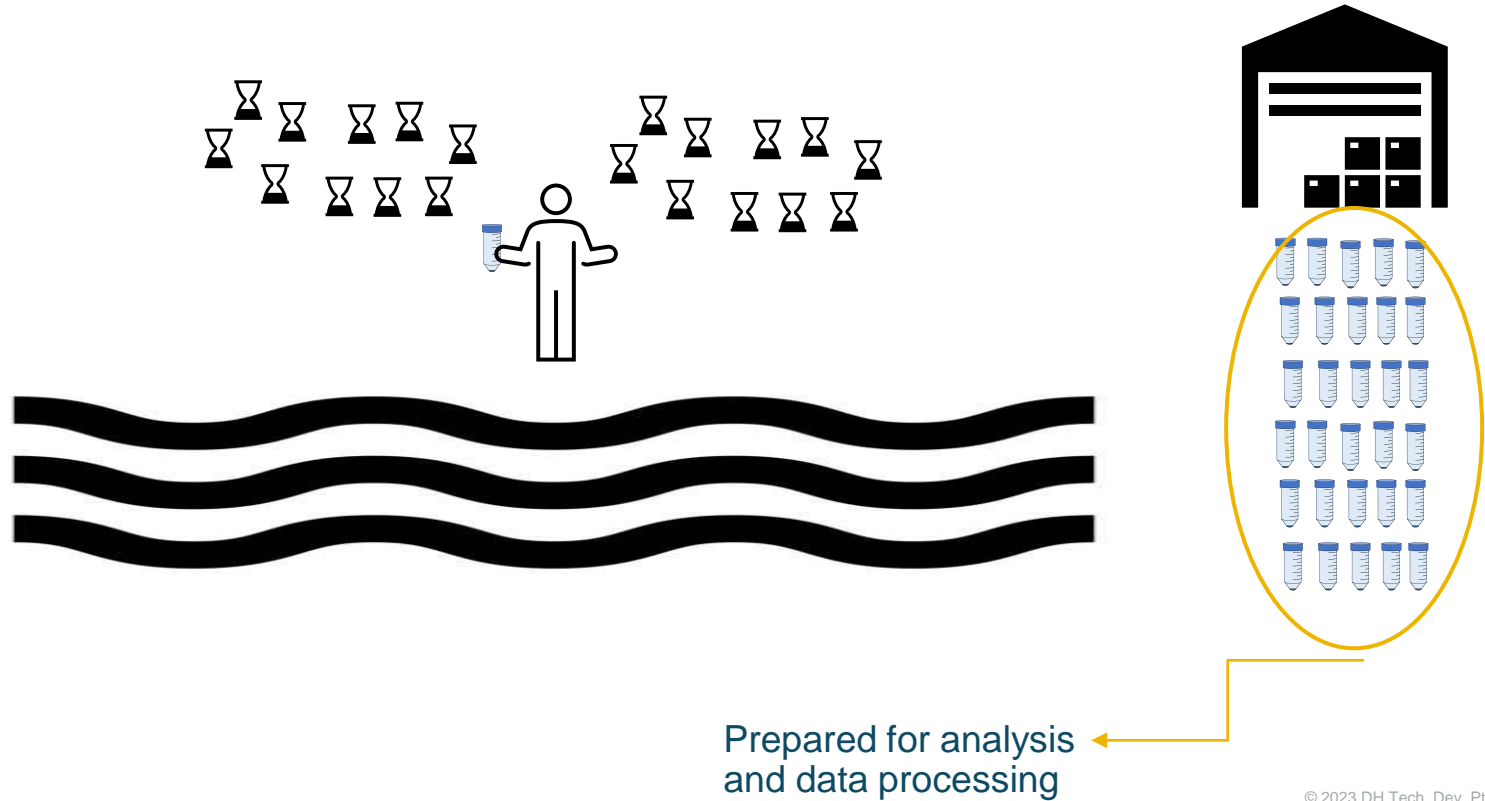
# Spatio-Temporal Monitoring



# Spatio-Temporal Monitoring



# Spatio-Temporal Monitoring





- Water sampled across various locations along this river used for drinking water across Europe
- LC-HRMS performed for data analysis, spiking with IS and analyzing a mixture of standards so quantitation and identification of unknowns can be performed
- enviMass used for prioritization and trend discovery
- Locations of identified compounds could be traced to industrial sources in those areas



Quantitative target and systematic non-target analysis of polar organic micro-pollutants along the river Rhine using high-resolution mass-spectrometry – Identification of unknown sources and compounds

Matthias Ruff, Miriam S. Mueller<sup>1</sup>, Martin Loos, Heinz P. Singer<sup>\*</sup>

*Eawag, Swiss Federal Institute of Aquatic Science and Technology, 8600 Dübendorf, Switzerland*

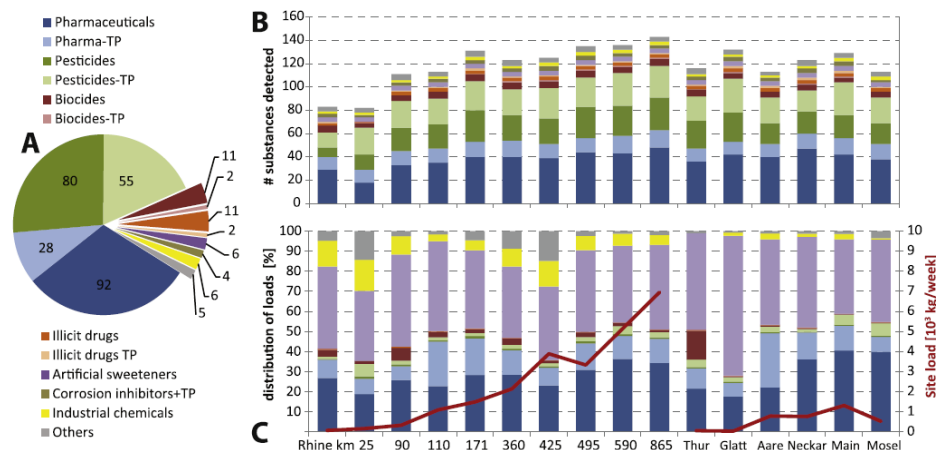


Fig. 2. A – Distribution of the investigated compounds grouped in substance classes; B – Number of substances detected at the sampling sites; C – Load distribution of the substance classes at each sampling site (left y-axis) and cumulative load of all quantifiable substances at each site (red curve on right y-axis). The color code of all graphs corresponds to legend 2A.

- The Lek River is a natural drinking water source and a branch of the Rhine River in The Netherlands
- Sampling of riverbank filtrate from a 60-year travel time
- Non-targeted MS analysis revealed trends over time maximized in the 1990s with increases in human activity, and wastewater treatment plant upgrades
- enviMass used for prioritization and ChemSpider utilized for structural ID

7  
published articles.

ENVIRONMENTAL  
Science & Technology

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Article

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## Nontarget Screening Reveals Time Trends of Polar Micropollutants in a Riverbank Filtration System

Vittorio Albergamo,<sup>\*,†</sup> Jennifer E. Schollée,<sup>‡</sup> Emma L. Schymanski,<sup>‡,§</sup> Rick Helmus,<sup>†</sup> Harrie Timmer,<sup>||</sup> Juliane Hollender,<sup>‡,†</sup> and Pim de Voogt<sup>†,¶</sup>

<sup>†</sup>Institute for Biodiversity and Ecosystem Dynamics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

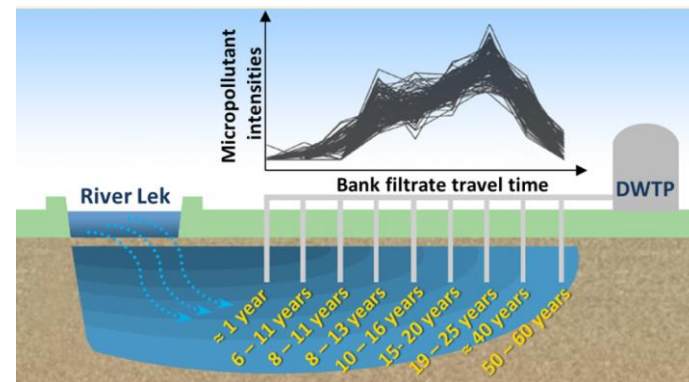
<sup>‡</sup>Eawag, Swiss Federal Institute of Aquatic Science and Technology, Überlandstrasse 133, 8600 Dübendorf, Switzerland

<sup>§</sup>Luxembourg Centre for Systems Biomedicine, University of Luxembourg, House of Biomedicine II 6, avenue du Swing, L-4367 Belvaux, Luxembourg

<sup>||</sup>Oasen, Nieuwe Gouwe O.Z. 3, 2801 SB Gouda, The Netherlands

<sup>‡</sup>Institute of Biogeochemistry and Pollutant Dynamics, ETH Zürich, Universitätsstrasse 16, 8092 Zürich, Switzerland

<sup>¶</sup>KWR Watercycle Research Institute, Groningenhaven 7, 3430 BB, Nieuwegein, The Netherlands



# HRMS for NTA



## Screening technique

## Question

**Nontarget analysis**

- Which compounds are present in this sample?
- *Known-unknowns and unknown-unknowns*

**Suspect screening**

- Which compounds of a defined list are present in this sample?
- *Known-unknowns*

**Targeted analysis**

- Are compounds x, y and z present in this sample?
- *Known-knowns*

## Difficulty



Hard

Moderate

Easy

## Time

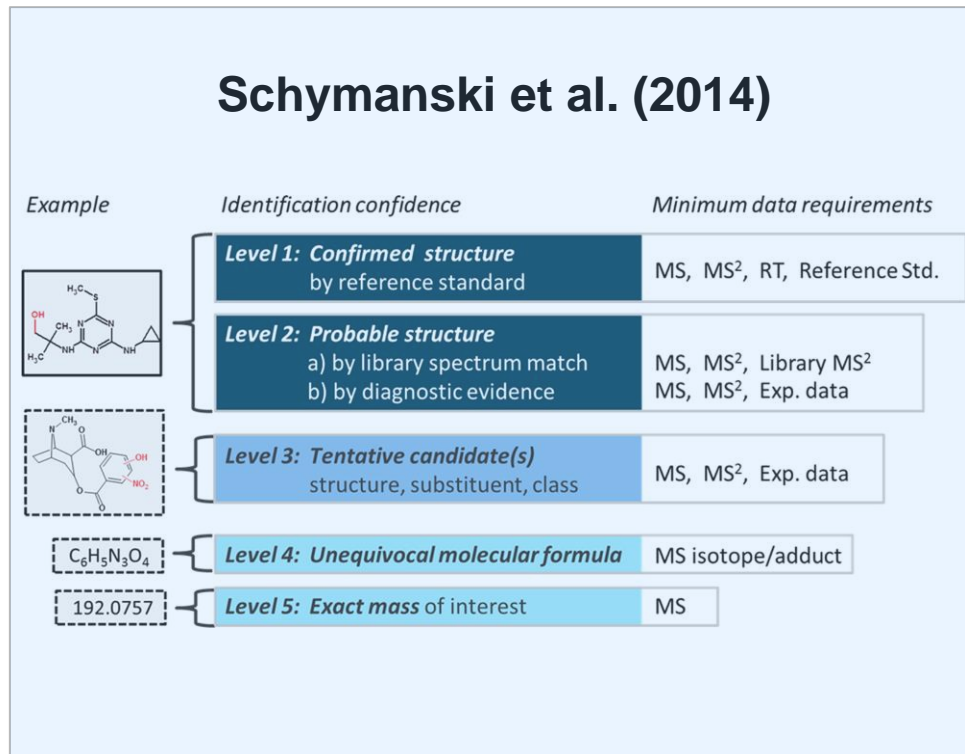


Weeks to months

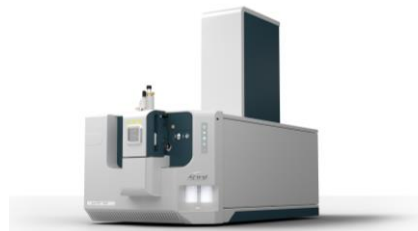
Days to weeks

Hours

The most-used ranking system in environmental analysis:



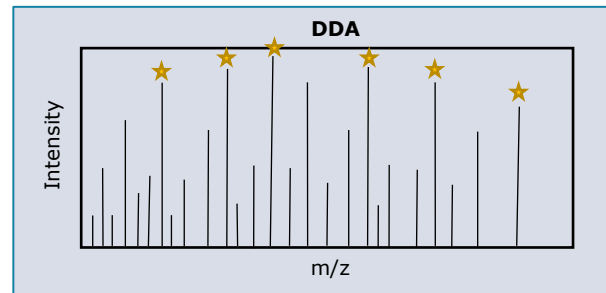
# HRMS data acquisition and workflows



Workflow	QTOF system
Traditional high selectivity quantitation	MRM <sup>HR</sup>
Suspect screening	MRM <sup>HR</sup> , SWATH DIA, DDA
Unknown screening	SWATH DIA, DDA

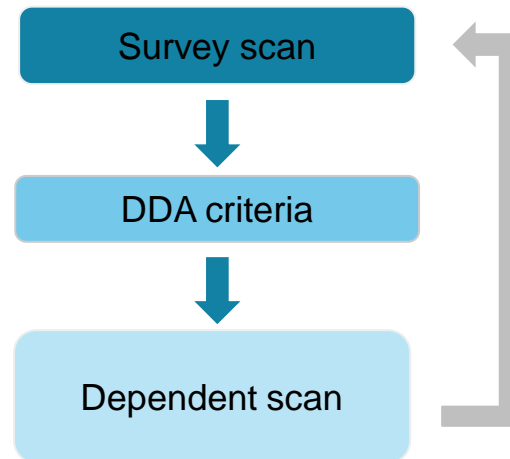
**Which compounds are present in this sample?**

Scan type	Meaning	Data dependent/ independent
DDA	Data dependent acquisition	Dependent
SWATH DIA	SWATH data independent acquisition	Independent



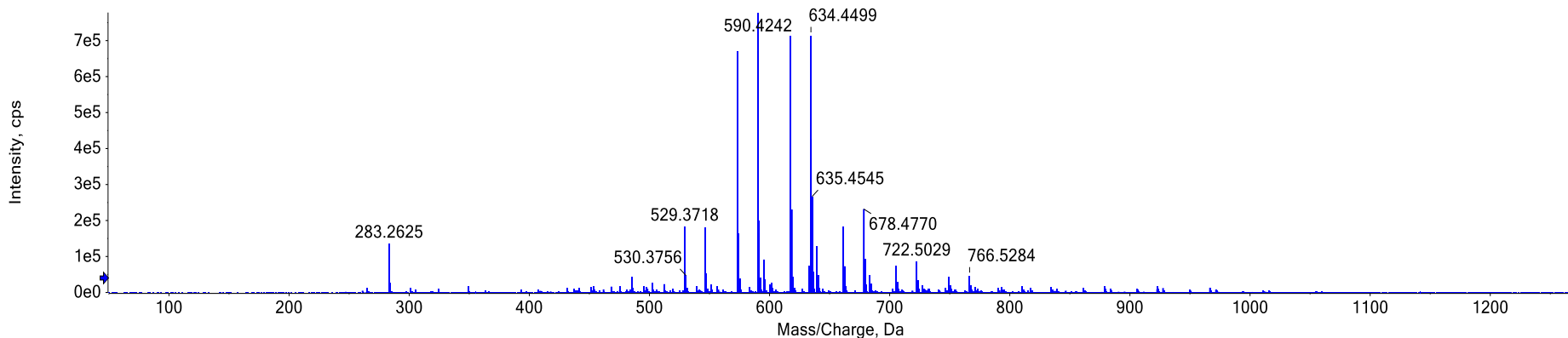
# Data dependent acquisition (DDA)

- DDA is an acquisition strategy that automatically selects candidate ions for MS/MS study
- First, a survey scan is performed (TOF MS)
- If any candidate ions acquired in the survey scan meet the DDA criteria, a dependent MS/MS experiment is initiated for qualifying candidates
- After all dependent scans are completed, the process repeats



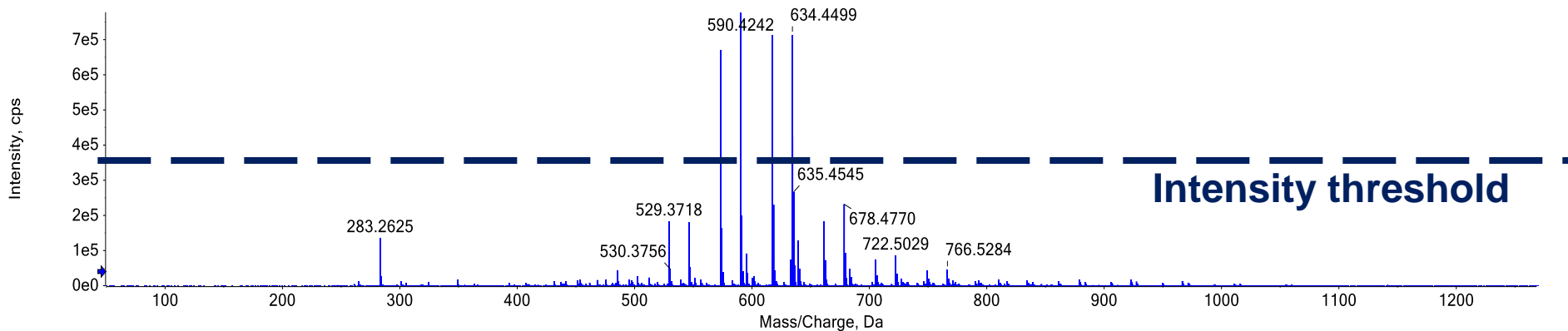


## Survey scan: TOF MS



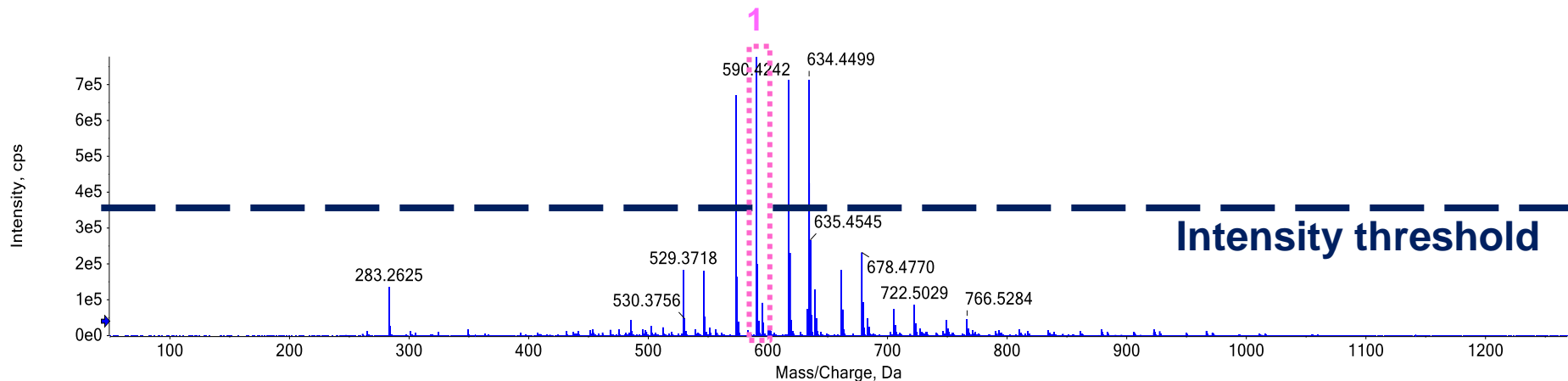
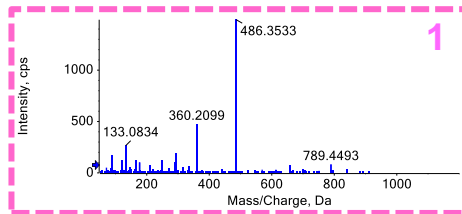
DDA criteria: select the top 10–12 most intense candidates

## Survey scan: TOF MS



DDA criteria: select the top 10–12 most intense candidates

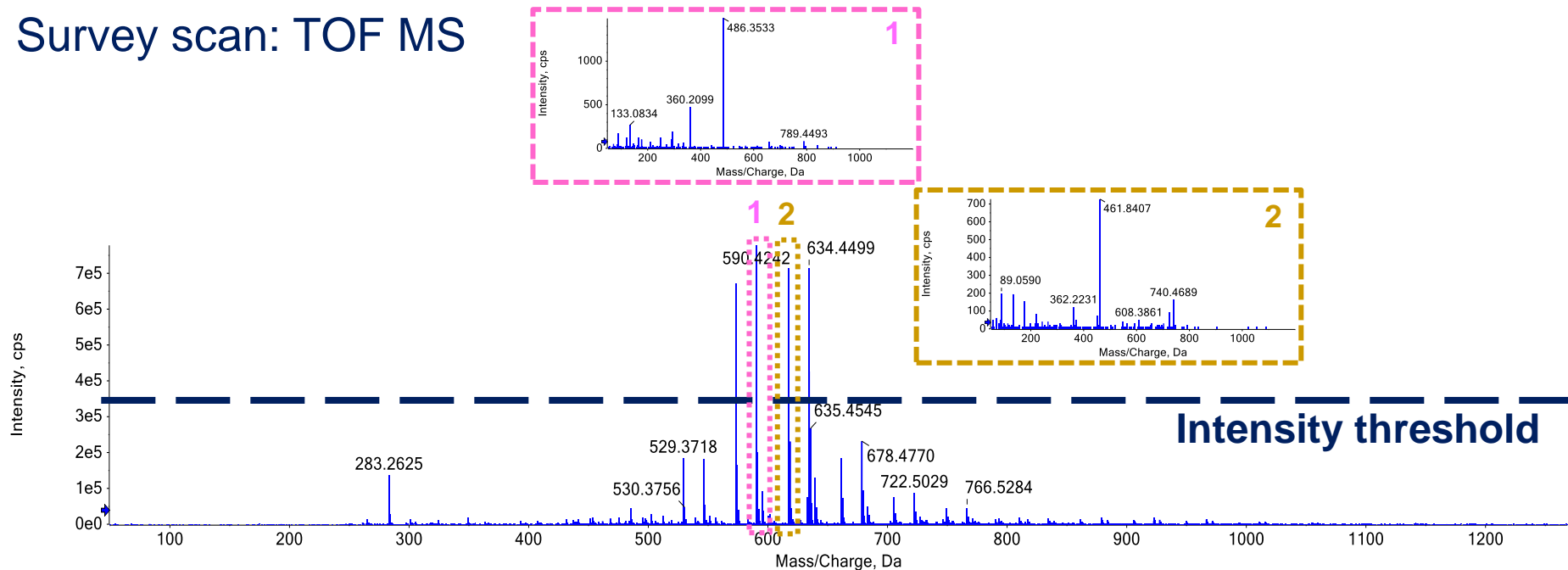
## Survey scan: TOF MS



DDA criteria: select the top 10–12 most intense candidates

# DDA overview

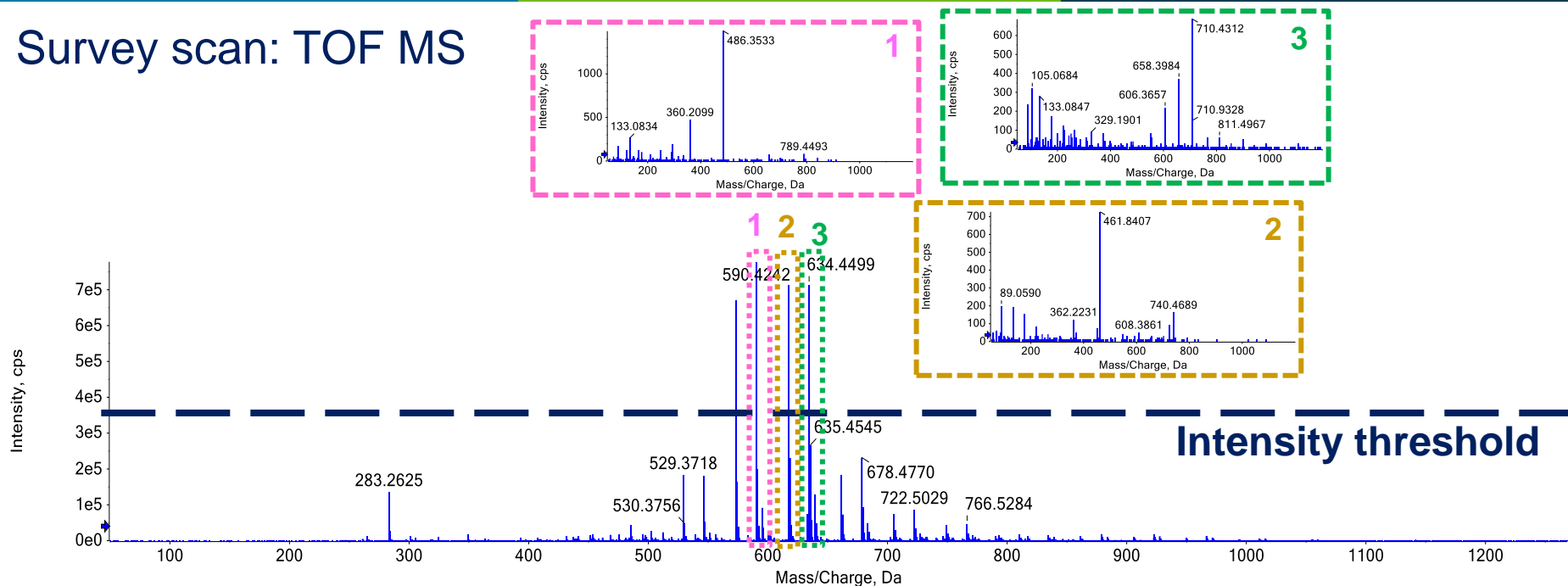
## Survey scan: TOF MS



DDA criteria: select the top 10–12 most intense candidates

# DDA overview

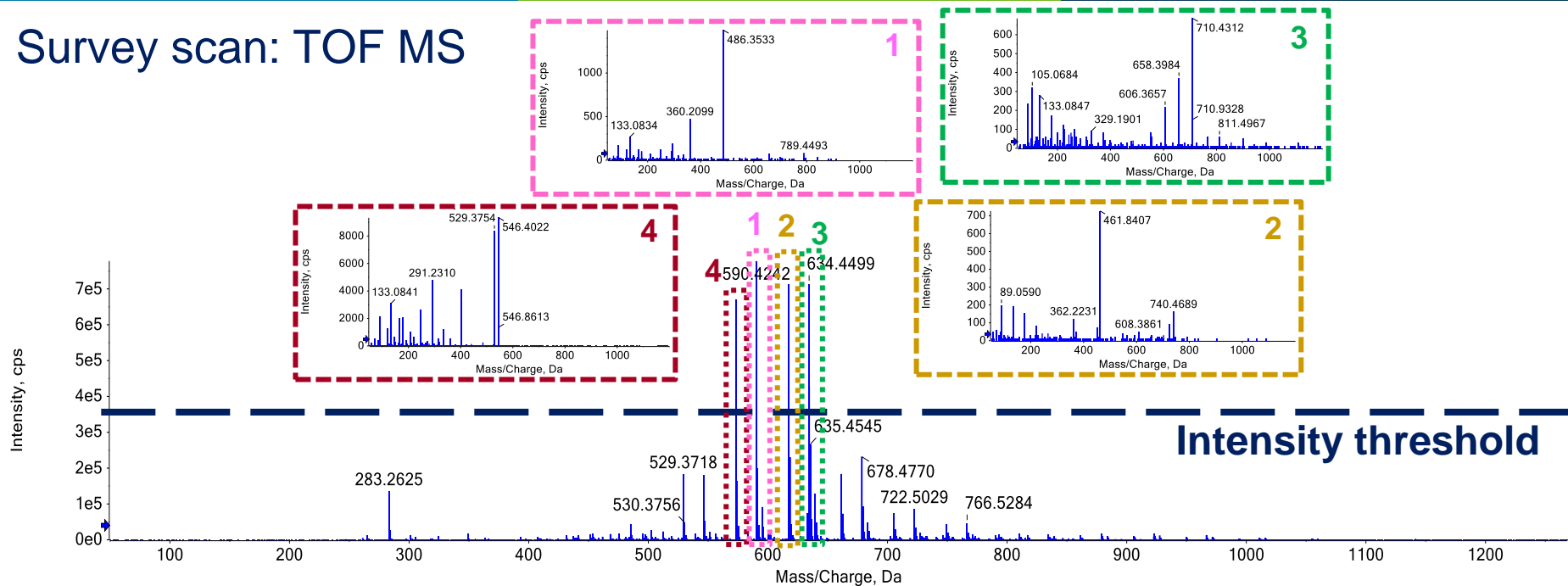
## Survey scan: TOF MS



DDA criteria: select the top 10–12 most intense candidates

# DDA overview

## Survey scan: TOF MS



DDA criteria: select the top 10–12 most intense candidates

# Our Water Study



# Sample Information

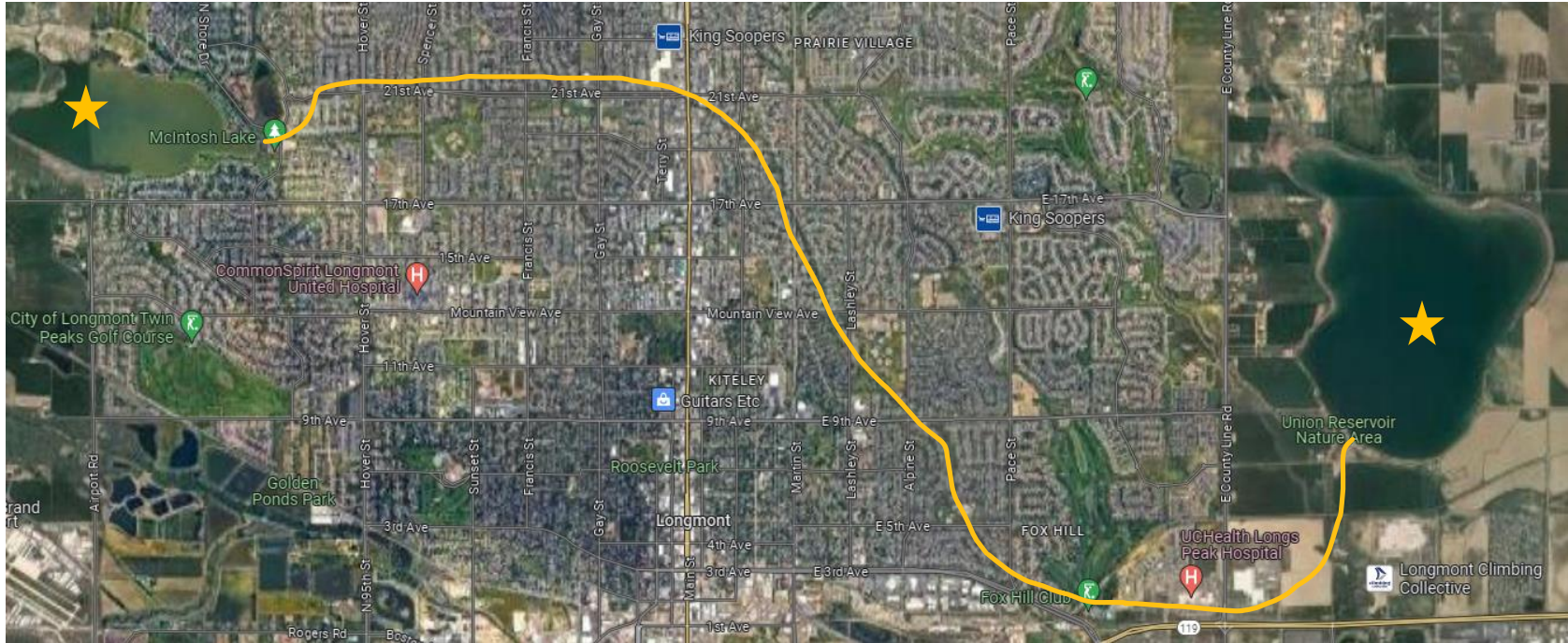
- Water source near Karl's house in Longmont, CO
  - Oligarchy Ditch runs from McIntosh Lake to Union Reservoir





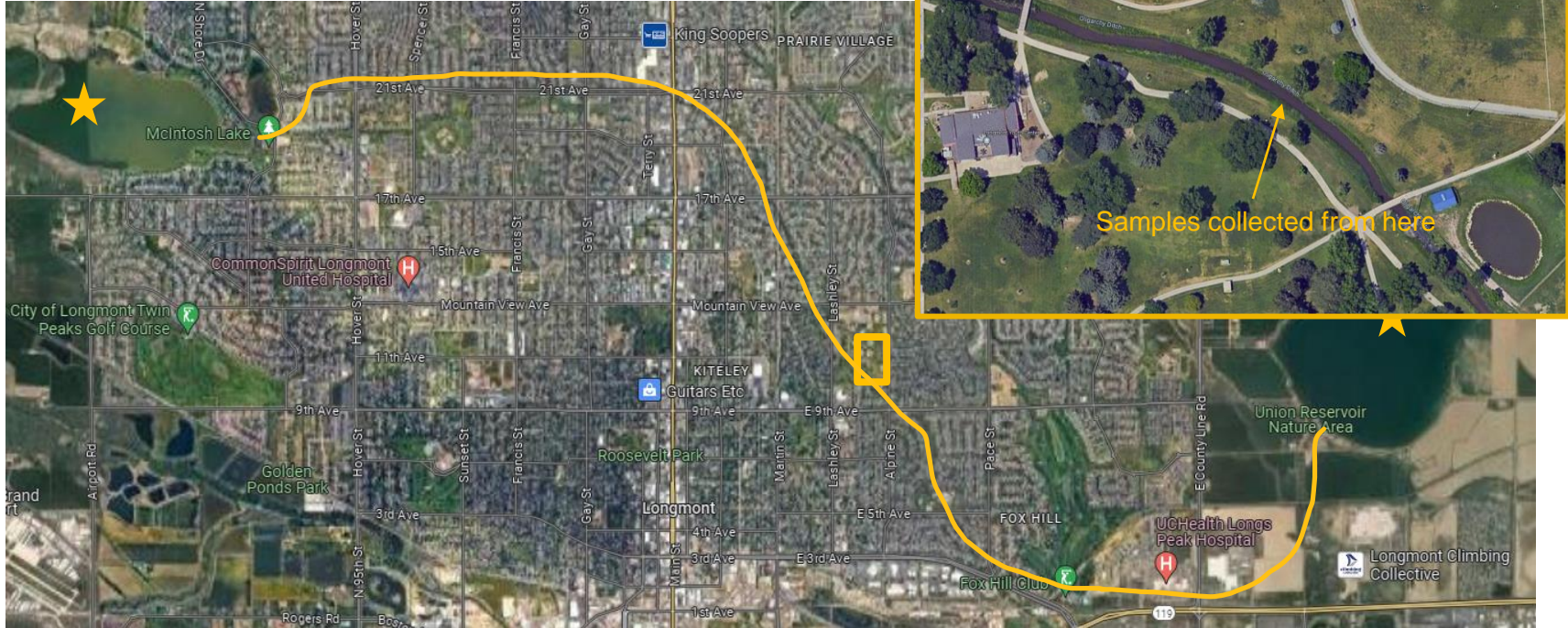
# Sample Information

## LONGMONT, CO



# Sample Information

## LONGMONT, CO WATER





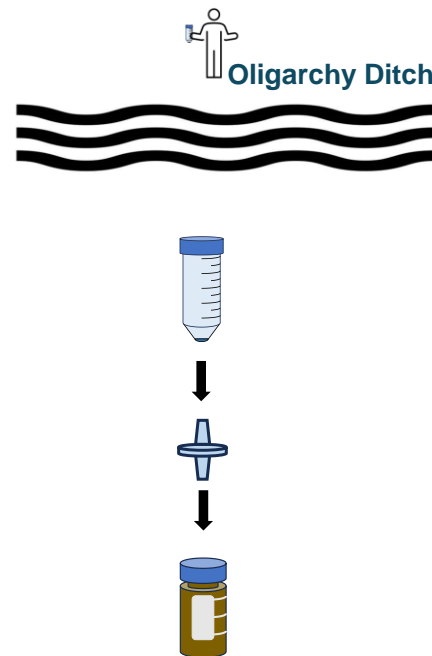
# Sample Information

- Water source near Karl's house
  - Oligarchy Ditch runs from McIntosh Lake to Union Reservoir
- Collected samples on a daily-ish basis across 1.5 months in the spring

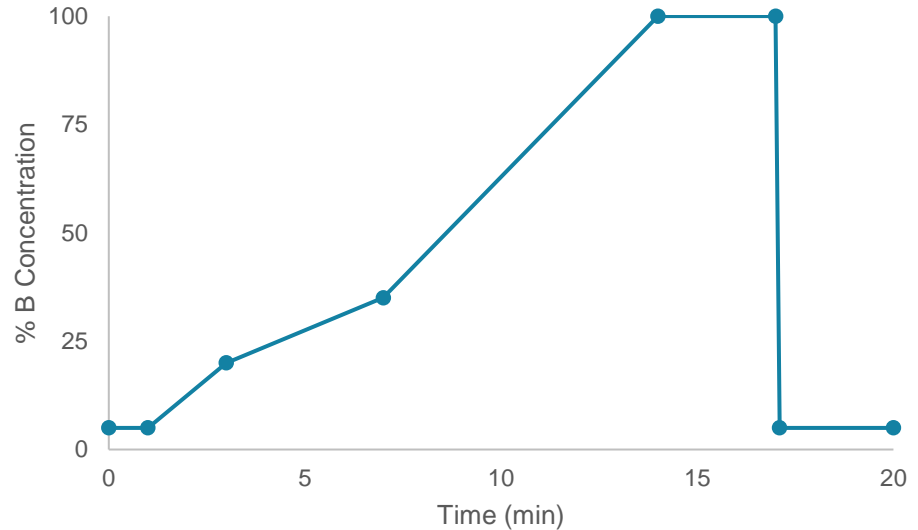


# Simple Sample Preparation

- Water samples were filtered using a 0.2  $\mu\text{m}$  nylon syringe filter directly to LC autosampler vial
- In this study we are only performing screening and identification, not quantification

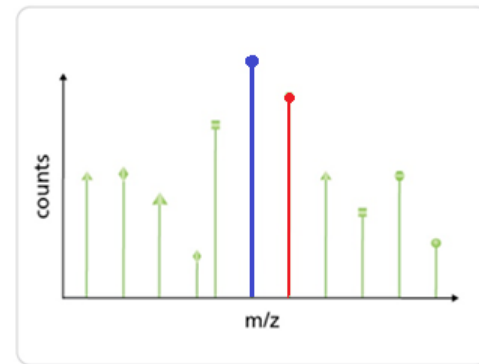
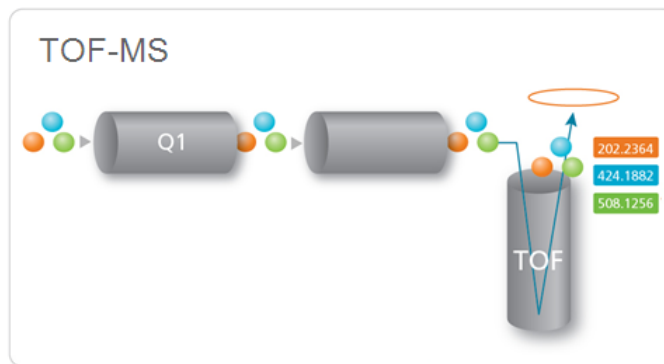


- Column: Phenomenex Luna Omega Polar C18 150 x 3 mm
- Flow rate: 0.7 mL/min
- Mobile phases
  - A: Water with 10mM ammonium formate and 0.1% formic acid
  - B: Acetonitrile with 10mM ammonium formate and 0.1% formic acid

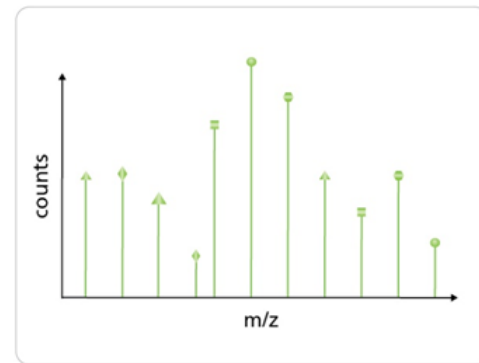
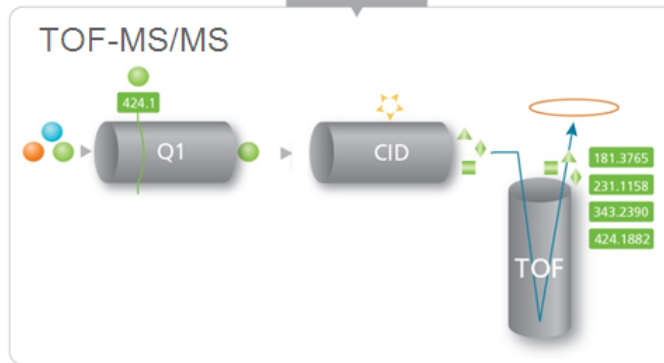


# ZenoTOF 7600 Analysis

- Data Dependent Analysis
- Top 14 candidate precursor ions
- Collision energy: 20 v
- Collision energy spread: 10 v



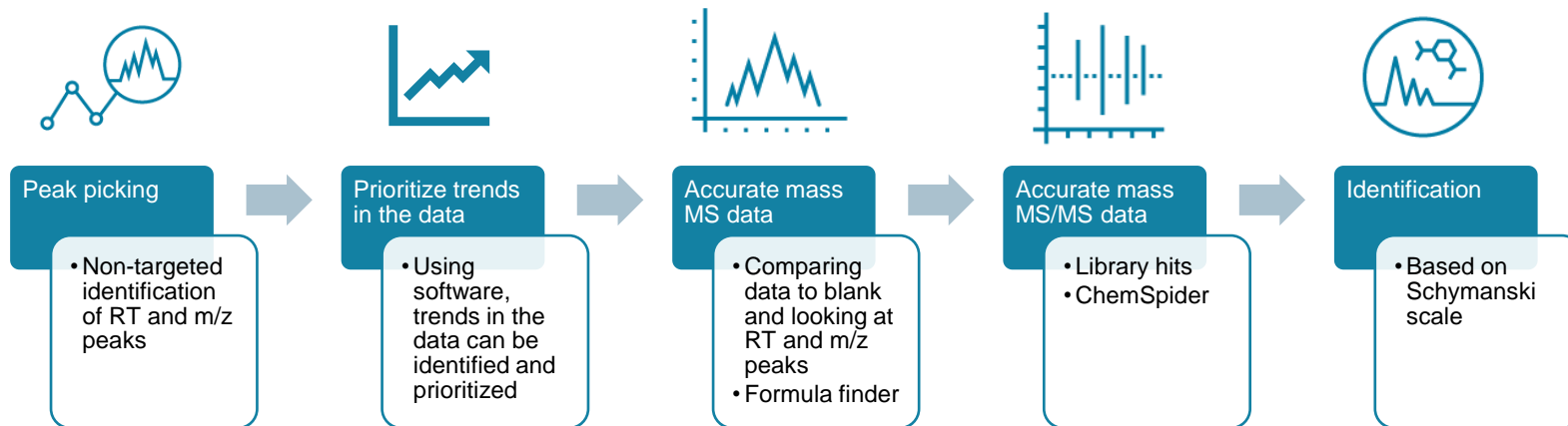
Criteria Pass



# Monitoring Trends



# Data processing workflow





# Non-Targeted Peak Picking

Configure the parameters to use to find the non-targeted peaks to add to the extracted ion chromatogram list

Minimum retention time  min

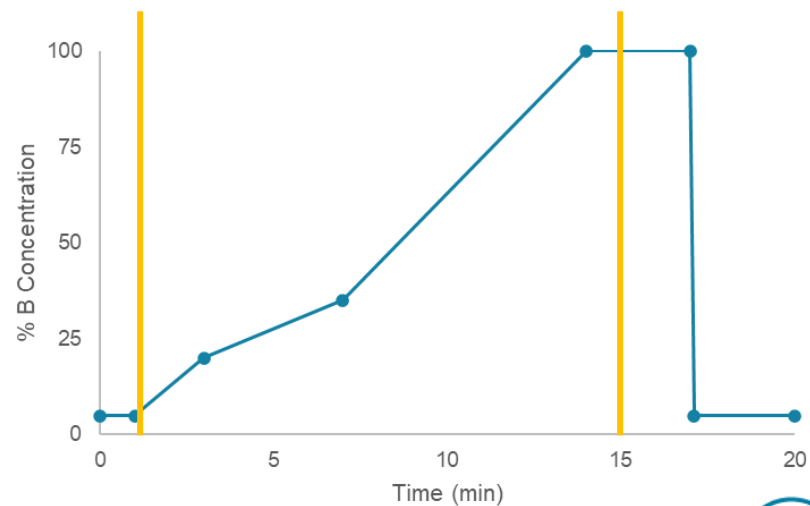
Maximum retention time  min

---

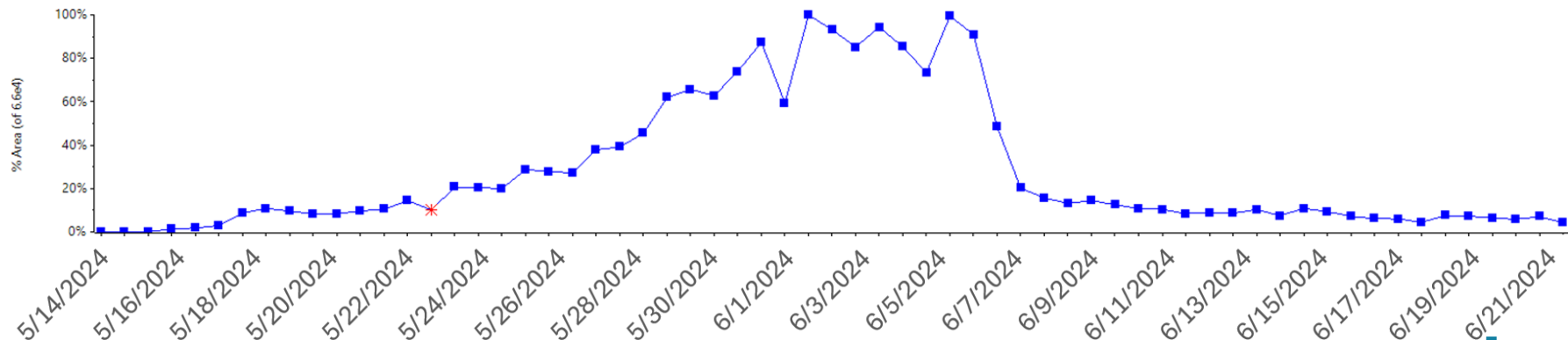
Peak detection sensitivity  Fast Exhaustive

Area Ratio Threshold (Unknown/Control)

Group peaks by adduct or charge

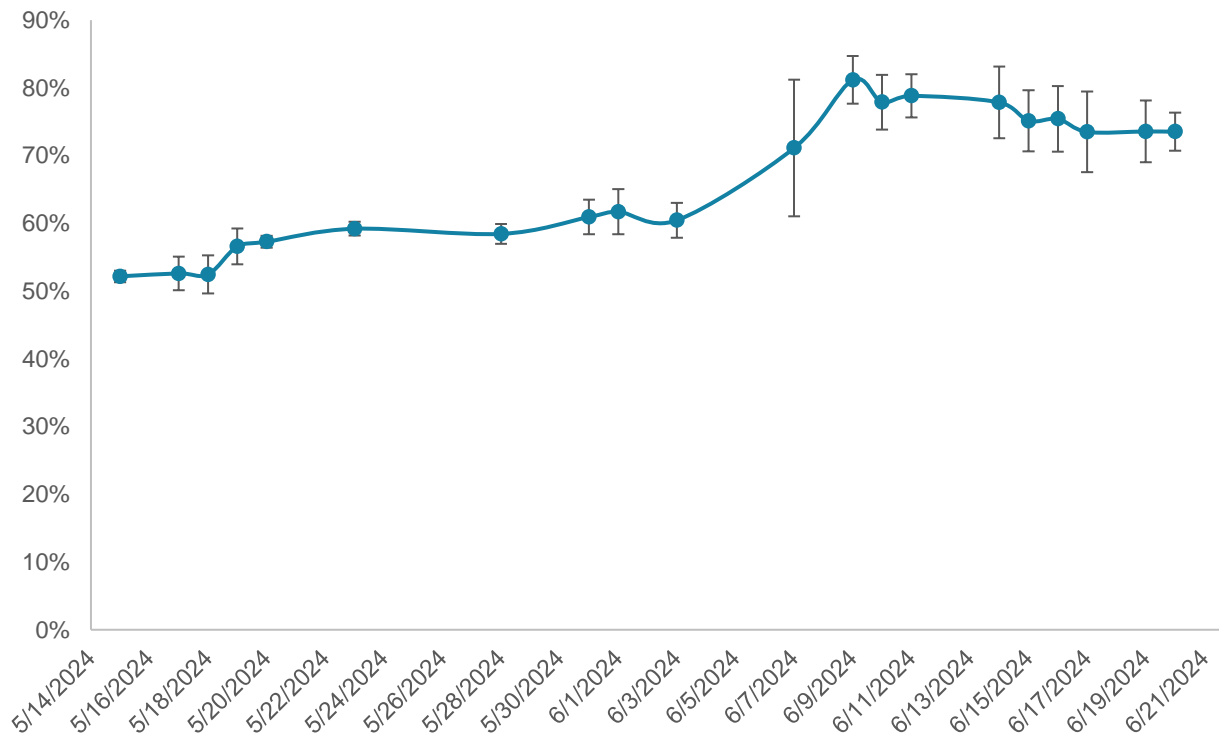


- Using enviMass for prioritization of untargeted data
- Unknown spectral features with distinct temporal trends were identified based on intensity patterns
- Using libraries and ChemSpider integrated into SciexOS to tentatively ID our prioritized compounds based on MS/MS fragmentation patterns and *in silico* fragmentation based on chemical structure



# Compound A

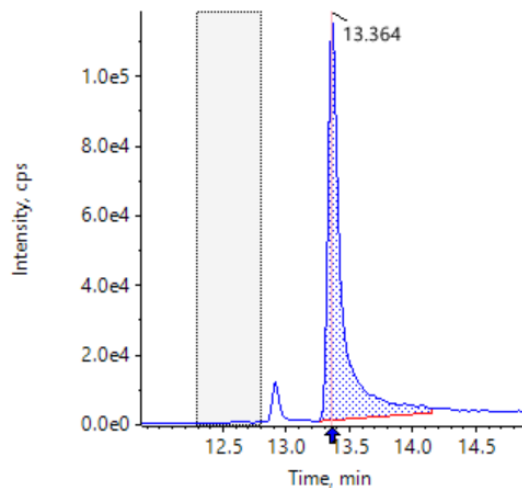
## Compound A: Normalized Area Over Time



# Compound A

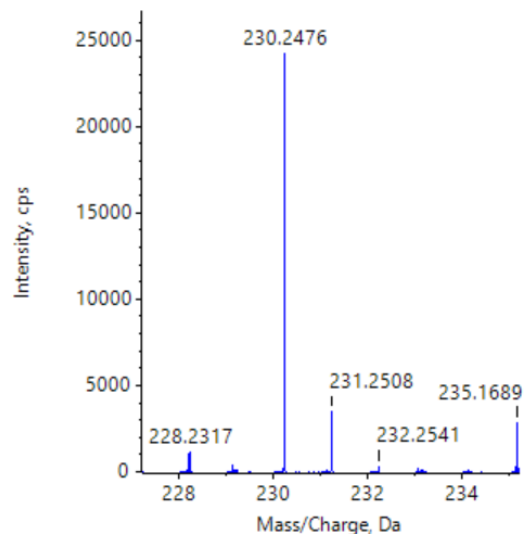
RT: 13.3 min  $m/z$ : 230.2476

617 - 230.2476 / 13.36 230.2375 - 230.2575  
Area: 8.835e5, Height: 1.172e5, RT: 13.36 min  
Noise Region Start-End: 12.29-12.79



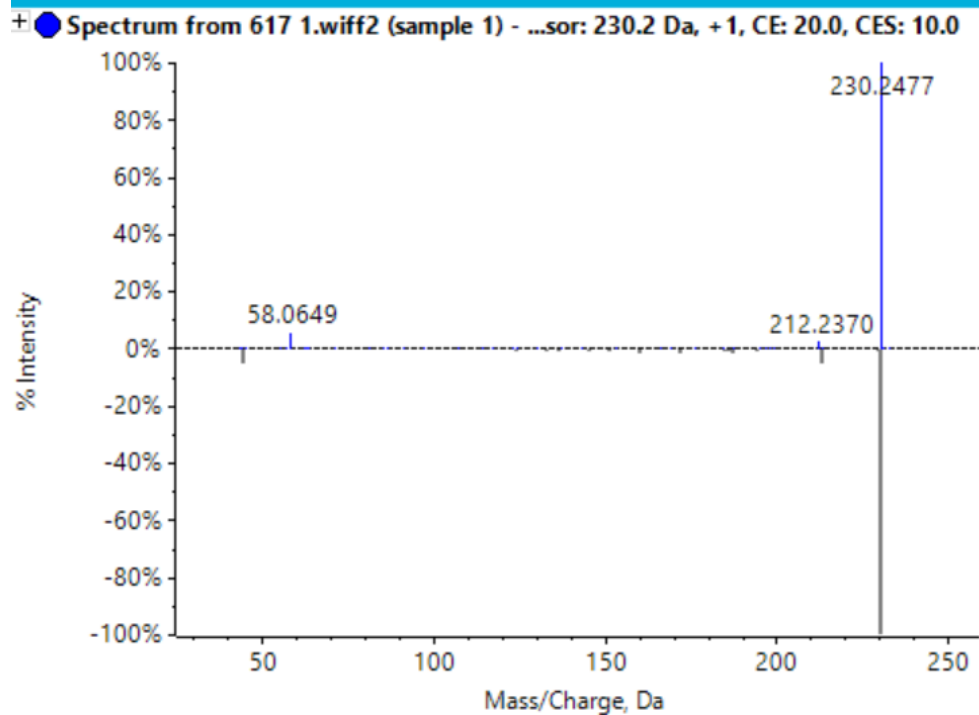
Extracted ion chromatogram

Spectrum from 617 1.wiff2 (s...) from 13.338 to 13.373 min



Precursor ion mass spectrum

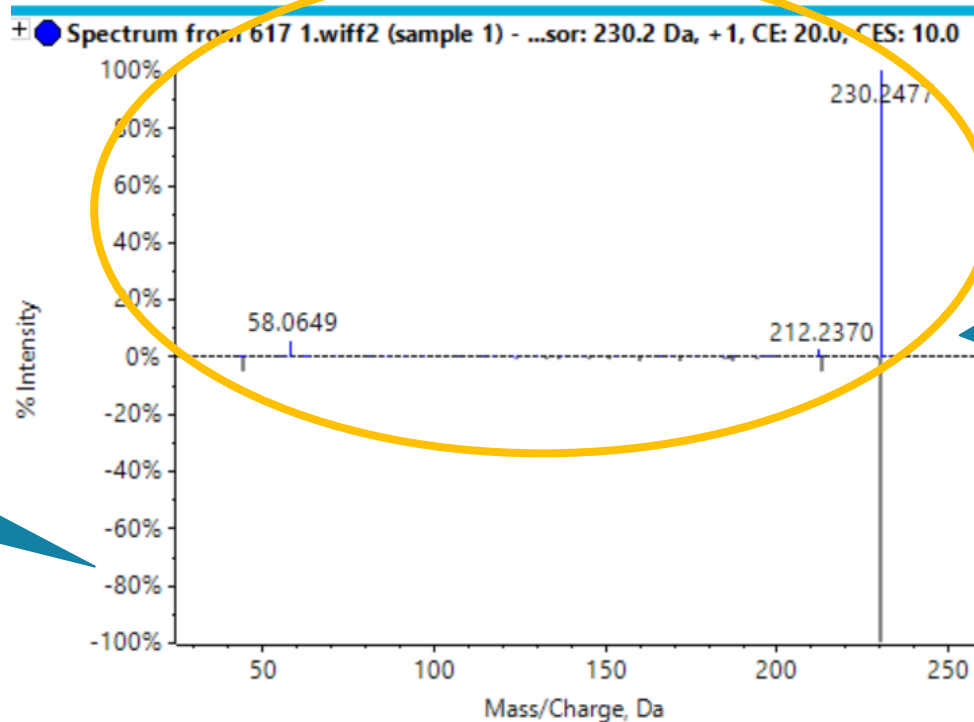




MS/MS Spectrum



# Compound A



Poor library matching

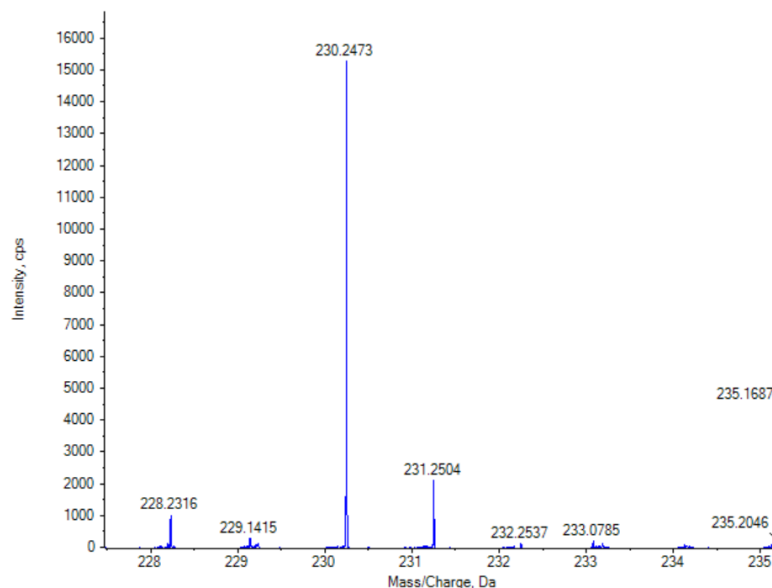
MS/MS spectrum lacking diagnostic fragmentation information

MS/MS Spectrum

# Compound A

- Using exact mass to match potential chemical formulas
- Searching ChemSpider Database for entries which match potential formula
- $C_{14}H_{31}NO$  matches the precursor molecular weight with a mass error of 2.4 ppm
  - ChemSpider produces >2000 hits in the database matching this formula

Spectrum from 620 3.wif#2 (sample 1) - 620, Experiment 1, +IDA TOF MS (100 - 2000) from 13.311 to 13.347 min

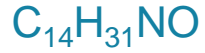


▲ Formula Finder Results

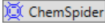
Name	Formula	Score	m/z (Da)	Error (ppm)	Error MSMS (ppm)	Hit Co
	C <sub>14</sub> H <sub>31</sub> NO	79.6	230.24784	2.4	1.4	2081




# Compound A



Compounds  
matching  
formula

ChemSpider results for:  $C_{14}H_{31}NO$   

1-40 of 2081 

CSID	Common Name	Molecular Weight
14688	Lauryldimethylamine oxide	229.402
77122	Dodecylethanolamine	229.402
23339950	xestoaminol C	229.402
2840262	3-(Undecylamino)-1-propanol	229.40204
13522586	1-Amino-2-tetradecanol	229.402
13789587	14-Amino-1-tetradecanol	229.402
3752270	MFCD04122509	229.40204
13332953	2-(Dodecyloxy)ethanamine	229.402
102501	2-Dodecanyl(dimethyl)amine oxide	229.402



# Compound A

## FORMULA FINDER AND CHEMSPIDER

Compounds  
matching  
formula

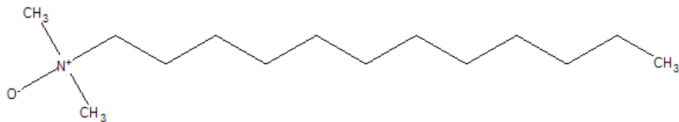
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Display all Carbon Atoms [Options...](#)

Structure of  
highlighted  
compound



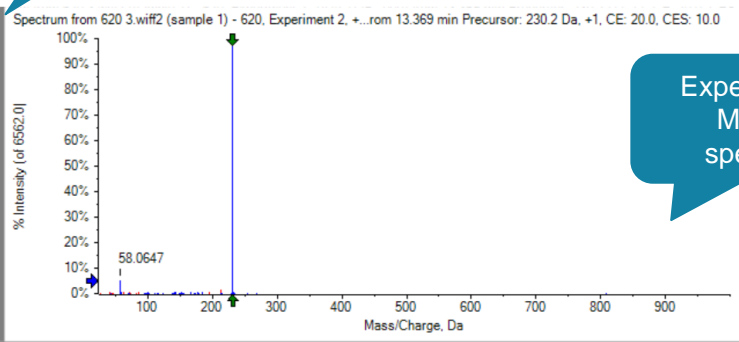
# Compound A

## FORMULA FINDER AND CHEMSPIDER

Compounds matching formula

ChemSpider results for: C14H31NO

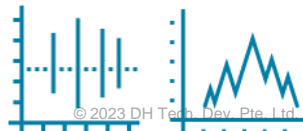
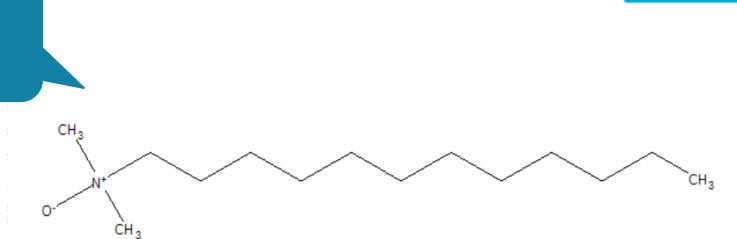
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13332953	2-(Dodecyl)ethanamine	229.402
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Experimental MS/MS spectrum

Structure of highlighted compound

Display all Carbon Atoms Options...



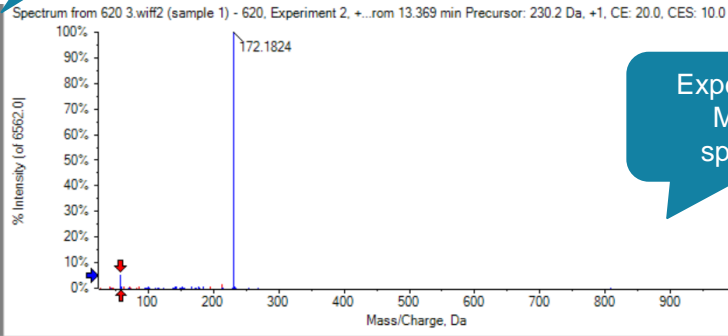
# Compound A

## FORMULA FINDER AND CHEMSPIDER

ChemSpider results for: C14H31NO

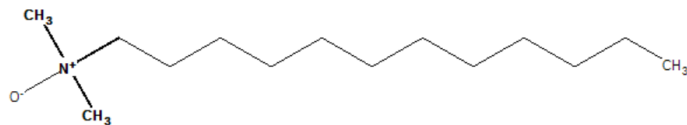
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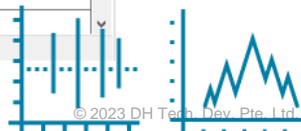


Options...

Mass/Charge	Intensity (%)	Assigned	Error (Da)
58.0647	5.39	<input checked="" type="checkbox"/>	0.000
230.0807	0.61	<input checked="" type="checkbox"/>	0.167
230.0888	0.32	<input checked="" type="checkbox"/>	0.159
230.1965	0.32	<input checked="" type="checkbox"/>	0.051
230.2475	100.00	<input checked="" type="checkbox"/>	0.000
230.2761	0.52	<input checked="" type="checkbox"/>	0.028
230.2943	0.56	<input checked="" type="checkbox"/>	0.046
230.5088	0.32	<input checked="" type="checkbox"/>	0.261
27.0219	0.30	<input type="checkbox"/>	

Matches: 8 of 27 peaks, 92.2% of total intensity

Fragments corresponding to structure



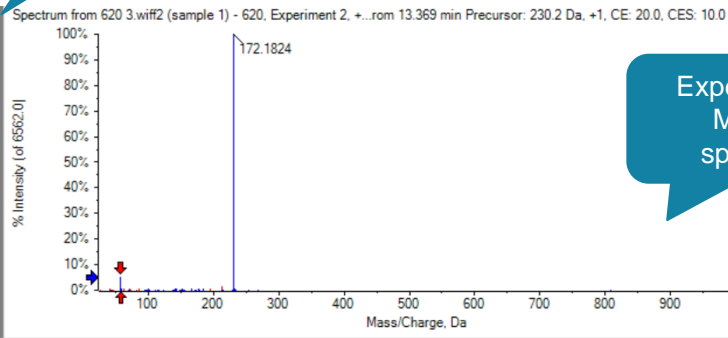
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## FORMULA FINDER AND CHEMSPIDER

ChemSpider results for: C<sub>14</sub>H<sub>31</sub>NO

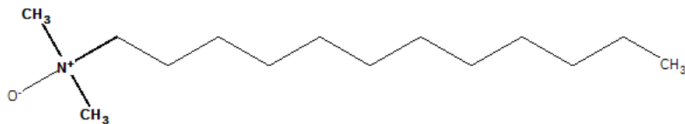
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Compounds matching formula



Experimental MS/MS spectrum

Structure of highlighted compound

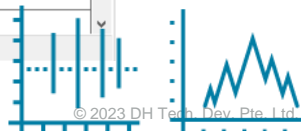


Options...

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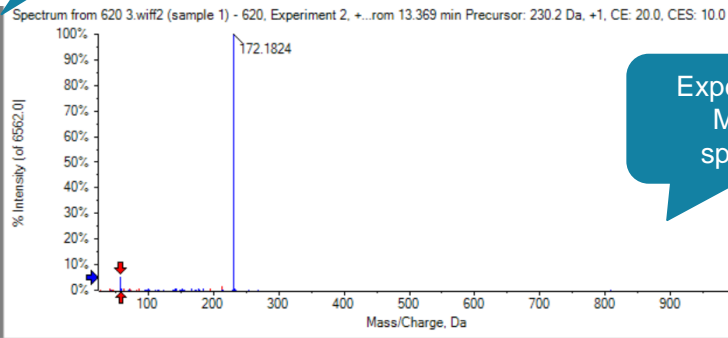
# Compound A

## FORMULA FINDER AND CHEMSPIDER

ChemSpider results for: C<sub>14</sub>H<sub>31</sub>N<sub>1</sub>O

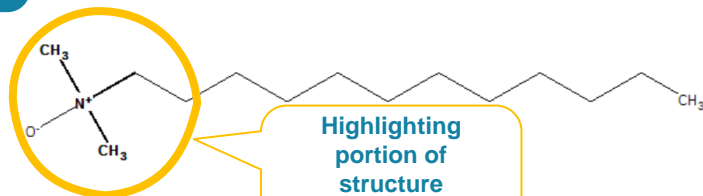
CSID	Common Name	Molecular Weight
14688	Lauryldimethylamine oxide	229.402
77122	Dodecylethanolamine	229.402
23339950	xestoaminol C	229.402
2840262	3-(Undecylamino)-1-propanol	229.40204
13522586	1-Amino-2-tetradecanol	229.402
13789587	14-Amino-1-tetradecanol	229.402
3752270	MFCD04122509	229.40204
13332953	2-(Dodecylloxy)ethanamine	229.402
102501	2-Dodecanyl(dimethyl)amine oxide	229.402

Compounds matching formula



Experimental MS/MS spectrum

Structure of highlighted compound

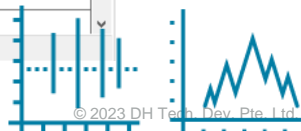


Highlighting portion of structure related to each fragment

Mass/Charge	Intensity (%)	Assigned	Error (Da)
58.0647	5.39	<input checked="" type="checkbox"/>	0.000
230.0807	0.61	<input checked="" type="checkbox"/>	0.167
230.0888	0.32	<input checked="" type="checkbox"/>	0.159
230.1965	0.32	<input checked="" type="checkbox"/>	0.051
230.2475	100.00	<input checked="" type="checkbox"/>	0.000
230.2761	0.52	<input checked="" type="checkbox"/>	0.028
230.2943	0.56	<input checked="" type="checkbox"/>	0.046
230.5088	0.32	<input checked="" type="checkbox"/>	0.261
27.0219	0.30	<input type="checkbox"/>	

Matches: 8 of 27 peaks, 92.2% of total intensity

Fragments corresponding to structure



# Compound A

## FORMULA FINDER AND CHEMSPIDER

Compounds  
matching

ChemSpider results for: C<sub>14</sub>H<sub>31</sub>N<sub>1</sub>O

1-40 of 2081

CSID	Common Name
14688	Lauryldimethylamine oxide
77122	Dodecylethanolamine
23339950	xestoaminol C
2840262	3-(Undecylamino)-1-propanol
13522586	1-Amino-2-tetradecanol
13789587	14-Amino-1-tetradecanol
3752270	MFCD04122509
13332953	2-(Dodecylloxy)ethanamine
102501	2-Dodecanyl(dimethyl)amine oxide

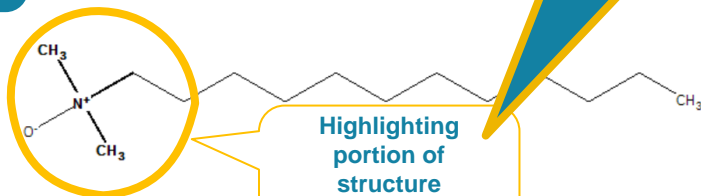
Level 3  
Identification with  
a tentative  
candidate structure

Experimental  
MS/MS  
spectrum

ment 2, +...rom 13.369 min Precursor: 230.2 Da, +1, CE: 20.0, CES: 10.0

Mass/Charge, Da

Structure of  
highlighted  
compound

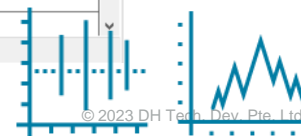


Highlighting  
portion of  
structure  
related to  
each fragment

Mass/Charge	Intensity (%)	Assigned	Error (Da)
58.0647	5.39	<input checked="" type="checkbox"/>	0.000
230.0807	0.61	<input checked="" type="checkbox"/>	0.167
230.0888	0.32	<input checked="" type="checkbox"/>	0.159
230.1965	0.32	<input checked="" type="checkbox"/>	0.051
230.2475	100.00	<input checked="" type="checkbox"/>	0.000
230.2761	0.52	<input checked="" type="checkbox"/>	0.028
230.2943	0.56	<input checked="" type="checkbox"/>	0.046
230.5088	0.32	<input checked="" type="checkbox"/>	0.261
27.0219	0.30	<input type="checkbox"/>	

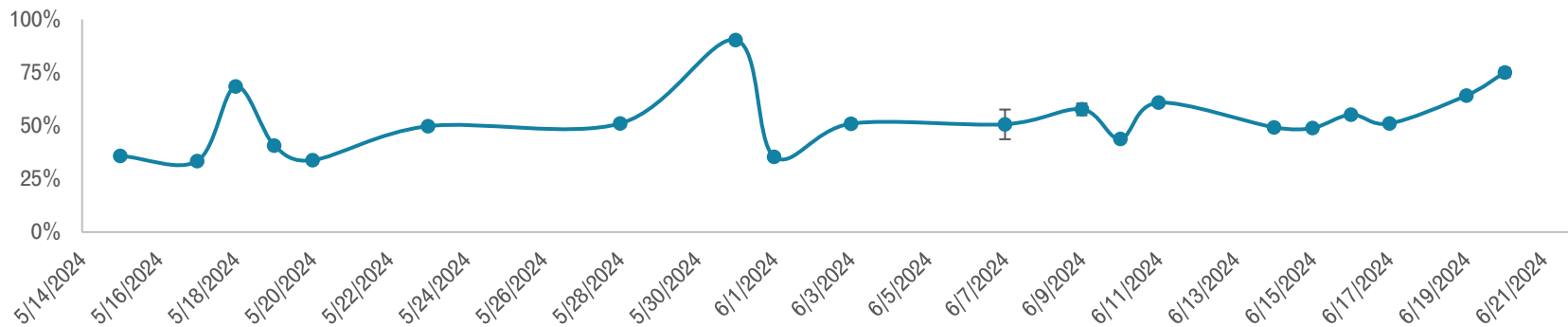
Matches: 8 of 27 peaks, 92.2% of total intensity

Fragments  
corresponding  
to structure

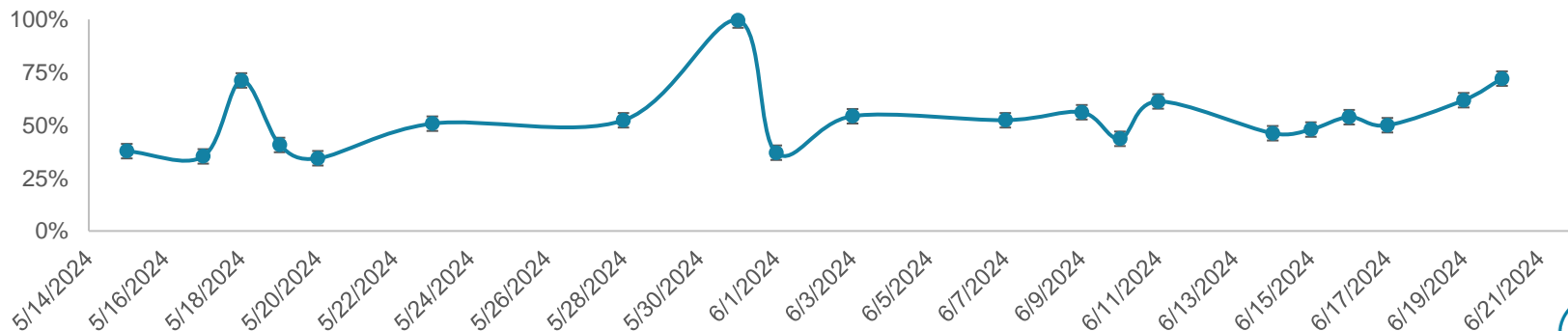


# Compound B

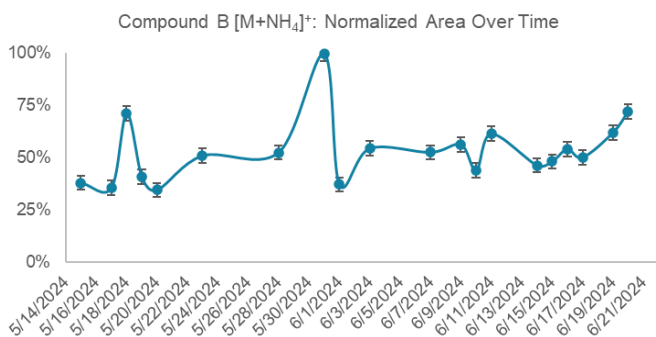
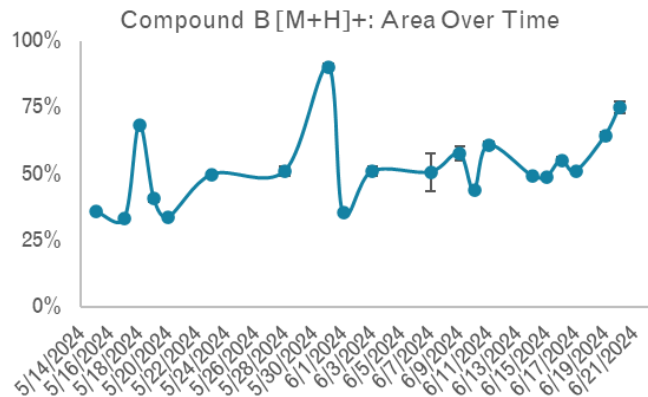
## Compound B [M+H]<sup>+</sup>: Area Over Time



## Compound B [M+NH<sub>4</sub>]<sup>+</sup>: Normalized Area Over Time



# Gage height trends



## ST Vrain CR Blw Boulder CR at Hwy 119 NR Longmont - 06730525

August 6, 2023 - August 5, 2024

Gage height, feet

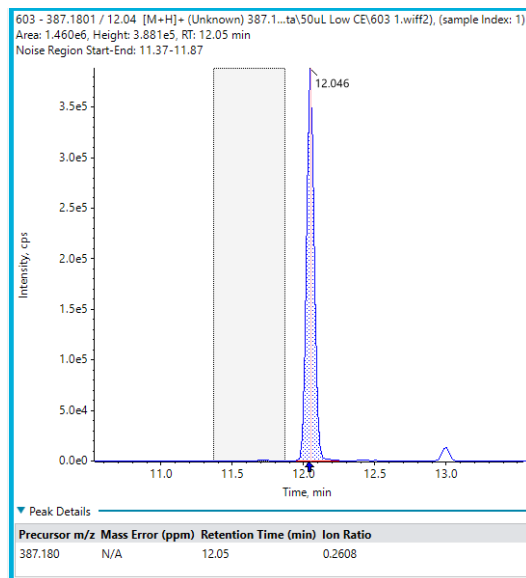
10.03 ft - May 14, 2024 05:00:00 AM MDT





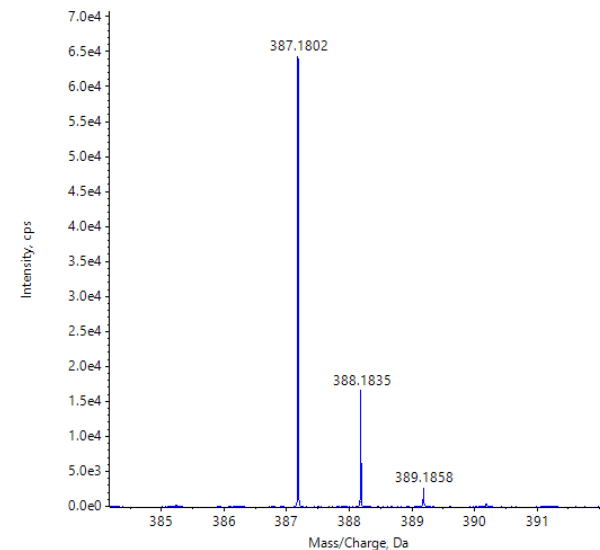
# Compound B

RT: 12.05 *m/z*: 387.1802



Extracted Ion Chromatogram  
Precursor Ion

Spectrum from 603 1.wiff2 (sample 1) - 603, Ex... TOF MS (100 - 2000) from 12.026 to 12.063 min

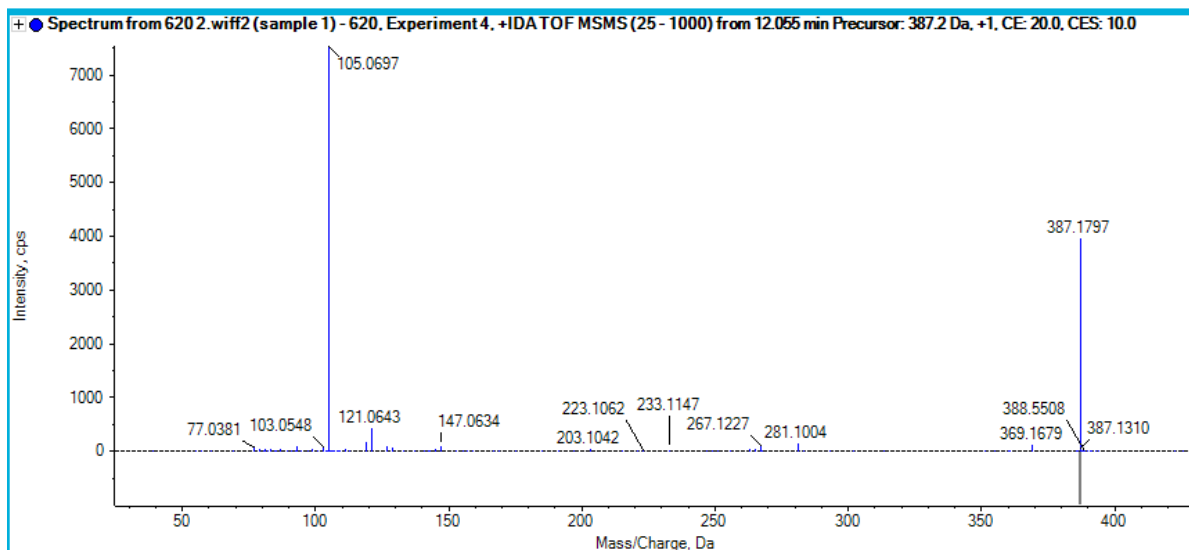


Extracted Ion Chromatogram  
Precursor Ion

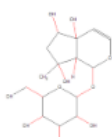


# MS/MS Spectrum Compound B

## LIBRARY MATCHES WITH LOW CONFIDENCE



### Library Search Results

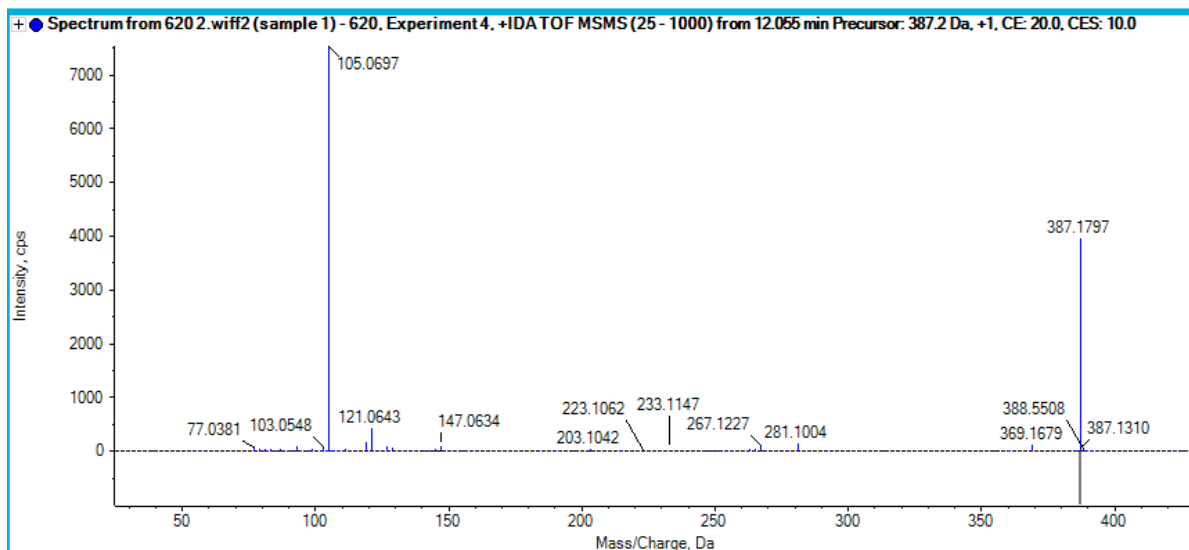


Name	CAS#	Formula	MM (Da)	Fit	Rev. Fit	Purity
Harpagide (NIST) [Smart Confirmation]	6926085	C <sub>15</sub> H <sub>24</sub> O <sub>10</sub>	364.13693	100.0	25.2	25.2
Dexanabinol (NIST) [Smart Confirmation]	112924455	C <sub>25</sub> H <sub>38</sub> O <sub>3</sub>	386.2821	63.0	73.6	20.6
15-Keto-17-phenyltrnorprostaglandin F2.alpha. (NIST) [Smart Confirmation]	949564890	C <sub>23</sub> H <sub>30</sub> O <sub>5</sub>	386.20932	11.9	100.0	11.9
Dexanabinol (NIST) [Smart Confirmation]	112924455	C <sub>25</sub> H <sub>38</sub> O <sub>3</sub>	386.2821	15.3	95.6	11.1

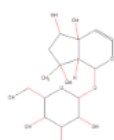


# MS/MS Spectrum Compound B

## LIBRARY MATCHES WITH LOW CONFIDENCE



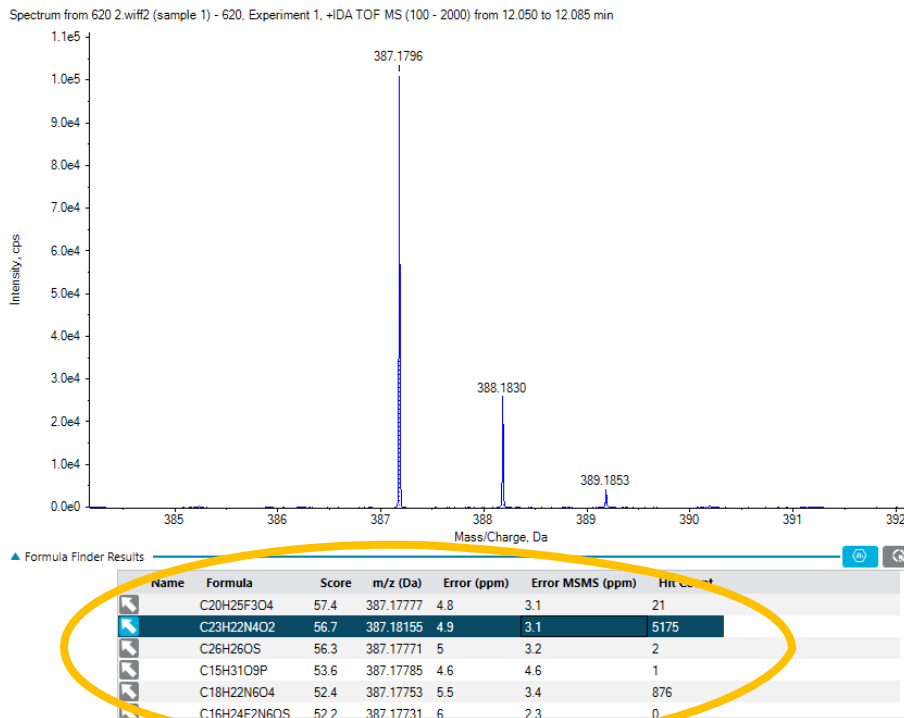
### ▲ Library Search Results



Name	CAS#	Formula	MM (Da)	Fit	Rev. Fit	Purity
Harpagide (NIST) [Smart Confirmation]	6926085	C <sub>15</sub> H <sub>24</sub> O <sub>10</sub>	364.13693	100.0	25.2	25.2
Dexanabinol (NIST) [Smart Confirmation]	112924455	C <sub>25</sub> H <sub>38</sub> O <sub>3</sub>	386.2821	63.0	73.6	20.6
15-Keto-17-phenyltrnorprostaglandin F2.alpha. (NIST) [Smart Confirmation]	949564890	C <sub>23</sub> H <sub>30</sub> O <sub>5</sub>	386.20932	11.9	100.0	11.9
Dexanabinol (NIST) [Smart Confirmation]	112924455	C <sub>25</sub> H <sub>38</sub> O <sub>3</sub>	386.2821	15.3	95.6	11.1



# Formula Finder Results





ChemSpider results for: C23H22N4O2

1-40 of 5175

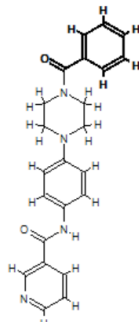


ChemSpider

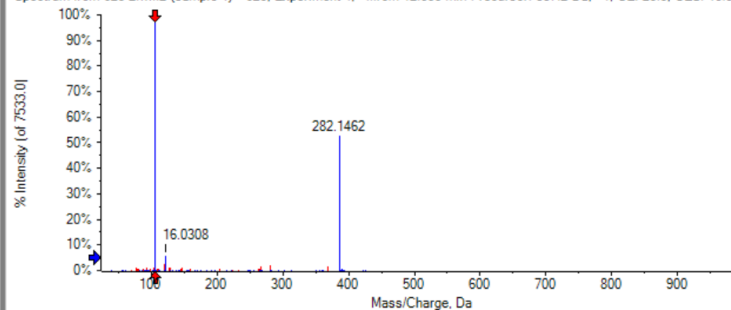
CSID	Common Name	Molecular Weight
2226208	2-(1,3-Benzoxazol-2-ylamino)-7,7-dimethyl-4-phenyl-4,6,7,8-tetrahydro-5(1H)-q	386.44638
2240915	5-[3-(Benzylamino)-2-hydroxypropyl]-3-methyl-1-oxo-1,5-dihydropyrido[1,2-a]	386.44638
2412972	N-[4-(4-Benzoyl-1-piperaziny)phenyl]nicotinamide	386.4464
2128322	1-(1-Naphthyl)-3-[4-(2-pyridinyl)-1-piperazinyl]-2,5-pyrrolidinedione	386.44638
2204962	N-[3-(1H-Imidazol-1-yl)propyl]-2-(3-methoxyphenyl)-4-quinolinecarboxamide	386.44638
2216888	6-Amino-4-(2-isopropoxyphenyl)-3-methyl-1-phenyl-1,4-dihydropyran[2,3-c]p	386.44638
2248274	N-(1-Cyclohexyl-1H-benzimidazol-5-yl)-2-(1H-indol-3-yl)-2-oxoacetamide	386.44638
1087624	N-[2-(4-Methoxyphenyl)-6-methyl-2H-benzotriazol-5-yl]-3,5-dimethylbenzamid	386.4464
4671877	6,6-Dimethyl-9-(3-phenoxyphenyl)-5,6,7,9-tetrahydro[1,2,4]triazolo[5,1-b]quinaz	386.4464

 Display all Carbon Atoms

Options...

selected composition: C<sub>7</sub>H<sub>3</sub>O<sup>+</sup> (105.0335 Da)

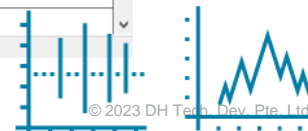
Spectrum from 620 2.wiff2 (sample 1) - 620, Experiment 4, +...rom 12.055 min Precursor: 387.2 Da, +1, CE: 20.0, CES: 10.0



Options...

Mass/Charge	Intensity (%)	Assigned	Error (Da)
105.0697	100.00	<input checked="" type="checkbox"/>	0.036
387.1797	52.54	<input checked="" type="checkbox"/>	0.002
121.0643	5.50	<input checked="" type="checkbox"/>	0.025
119.0487	2.28	<input type="checkbox"/>	
281.1004	1.87	<input type="checkbox"/>	
369.1679	1.66	<input type="checkbox"/>	
267.1227	1.45	<input type="checkbox"/>	
147.0634	1.19	<input type="checkbox"/>	
103.0548	1.14	<input type="checkbox"/>	

Matches: 11 of 48 peaks, 87.1% of total intensity

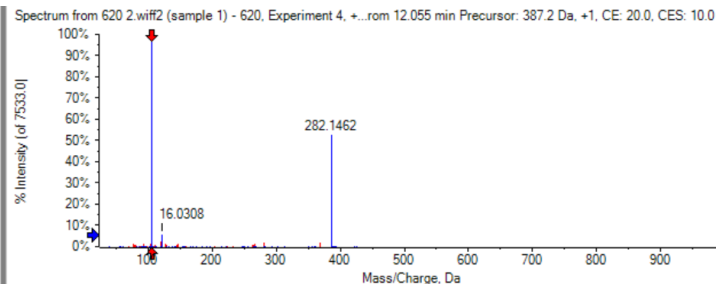




ChemSpider results for: C22H26O6

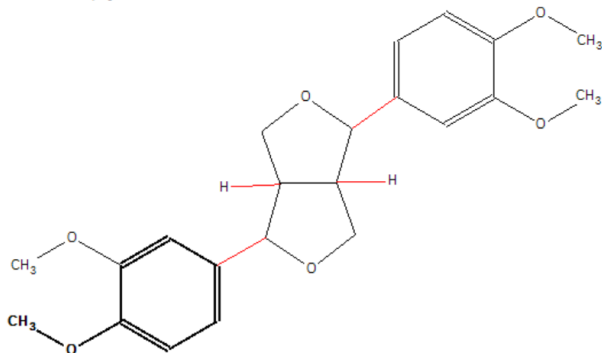
1-40 of 658

CSID	Common Name	Molecular Weight
65896	(+)-Eudesmin	386.4382
77441	benzophenone, 2-(1-ethylacetyl)-3',4',5-tetramethoxy-	386.4382
28530778	Tofogliflozin	386.4382
4479005	Gomisin M1	386.4382
5254121	1,3:2,4-Di-p-methylbenzylidene sorbitol	386.43824
341038	DIMETHYLMATAIRESINOL	386.4382
288301	eudesmin	386.4382
204828	1,4-Bis(3,4-dimethoxyphenyl)tetrahydro-1H,3H-furo[3,4-c]furan	386.4382



Display all Carbon Atoms

selected composition: C<sub>7</sub>H<sub>5</sub>O<sup>+</sup> (105.0335 Da)



Mass/Charge	Intensity (%)	Assigned	Error (Da)
105.0697	100.00	<input checked="" type="checkbox"/>	0.036
387.1797	52.54	<input checked="" type="checkbox"/>	0.001
121.0643	5.50	<input checked="" type="checkbox"/>	0.036
119.0487	2.28	<input type="checkbox"/>	
281.1004	1.87	<input type="checkbox"/>	
369.1679	1.66	<input type="checkbox"/>	
267.1227	1.45	<input type="checkbox"/>	
147.0634	1.19	<input type="checkbox"/>	
103.0548	1.14	<input type="checkbox"/>	
127.0376	1.12	<input type="checkbox"/>	

Matches: 11 of 48 peaks, 87.1% of total intensity

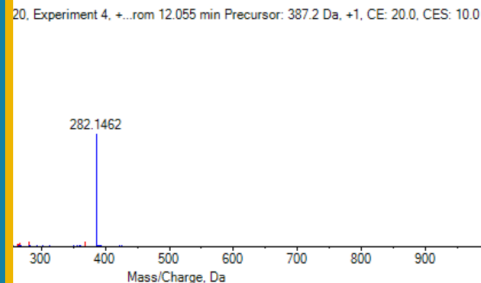
## ALTERNATIVE FORMULA

ChemSpider results for: C<sub>22</sub>H<sub>26</sub>O<sub>6</sub> F

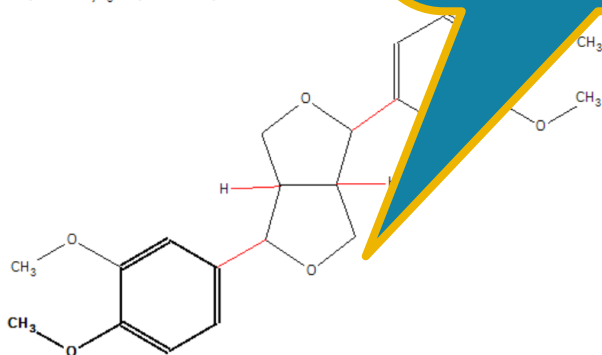
1-40 of 658

CSID	Common Name
65896	(+)-Eudesmin
77441	benzophenone, 2-(1-ethylacetyl)-3',4',5-tetramethoxy-
28530778	Tofogliflozin
4479005	Gomisin M1
5254121	1,3:2,4-Di-p-methylbenzylidene sorbitol
341038	DIMETHYLMATAIRESINOL
288301	eudesmin
204828	1,4-Bis(3,4-dimethoxyphenyl)tetrahydro-1H,3H-furo[3,4-

**Level 5  
Identification with  
exact mass only**

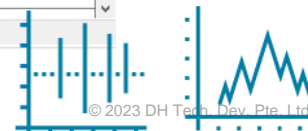


selected composition: C<sub>7</sub>H<sub>5</sub>O<sup>+</sup> (105.0335 Da)



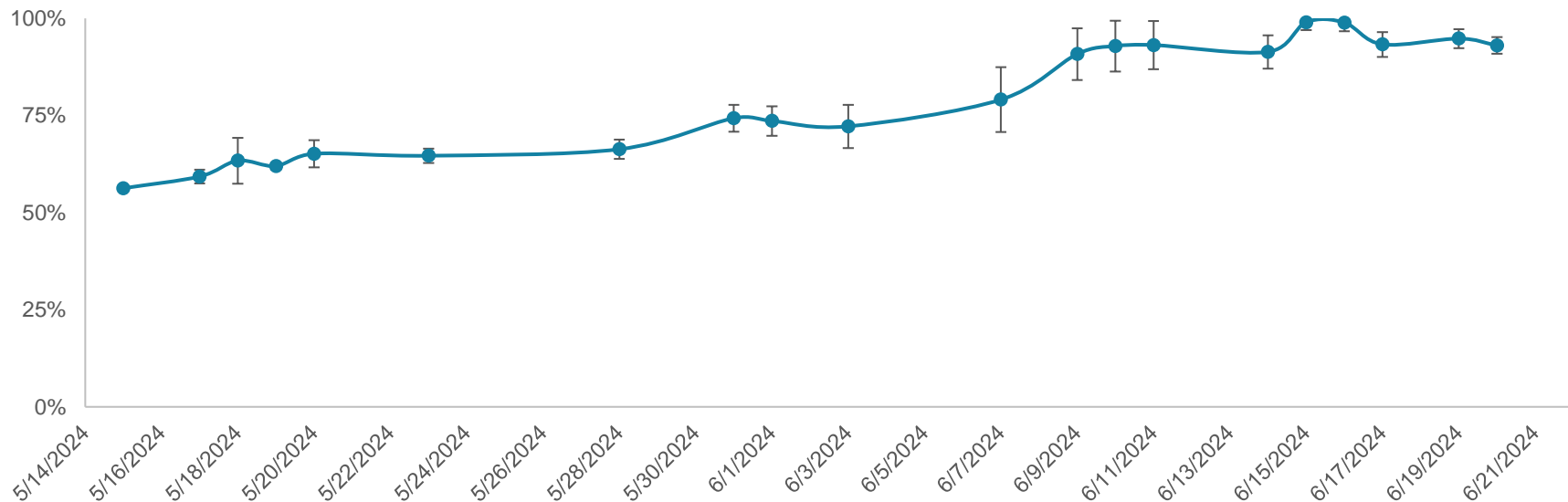
Mass/Charge	Intensity (%)	Assigned	Error (Da)
105.0697	100.00	<input checked="" type="checkbox"/>	0.036
387.1797	52.54	<input checked="" type="checkbox"/>	0.001
121.0643	5.50	<input checked="" type="checkbox"/>	0.036
119.0487	2.28	<input type="checkbox"/>	
281.1004	1.87	<input type="checkbox"/>	
369.1679	1.66	<input type="checkbox"/>	
267.1227	1.45	<input type="checkbox"/>	
147.0634	1.19	<input type="checkbox"/>	
103.0548	1.14	<input type="checkbox"/>	
127.0376	1.12	<input type="checkbox"/>	
63.0627	1.00	<input type="checkbox"/>	

Matches: 11 of 48 peaks, 87.1% of total intensity



# Compound C

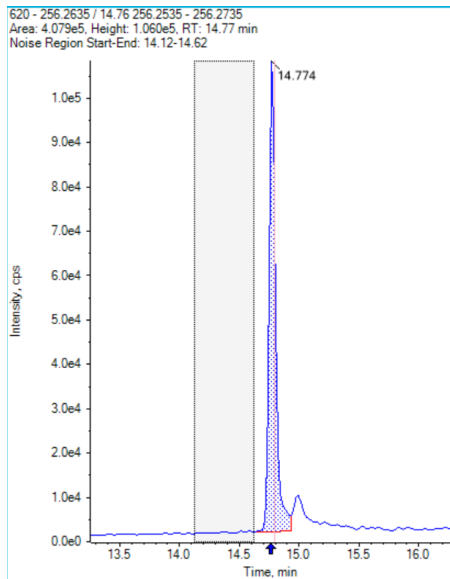
### Compound C: Normalized Area Over Time





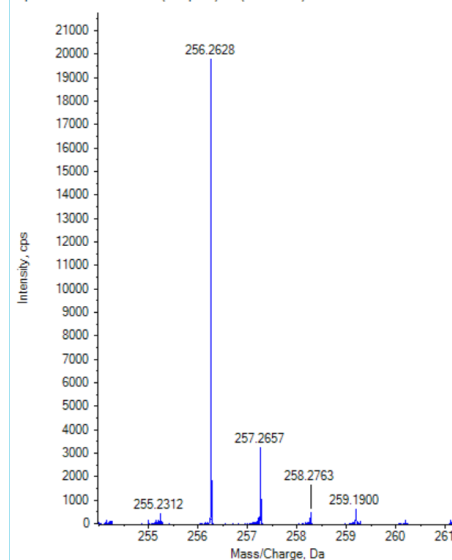
# Compound C

RT: 14.77  $m/z$  256.2628



Extracted ion chromatogram

Spectrum from 620 2.wiff2 (sample 1) - ... (100 - 2000) from 14.751 to 14.788 min

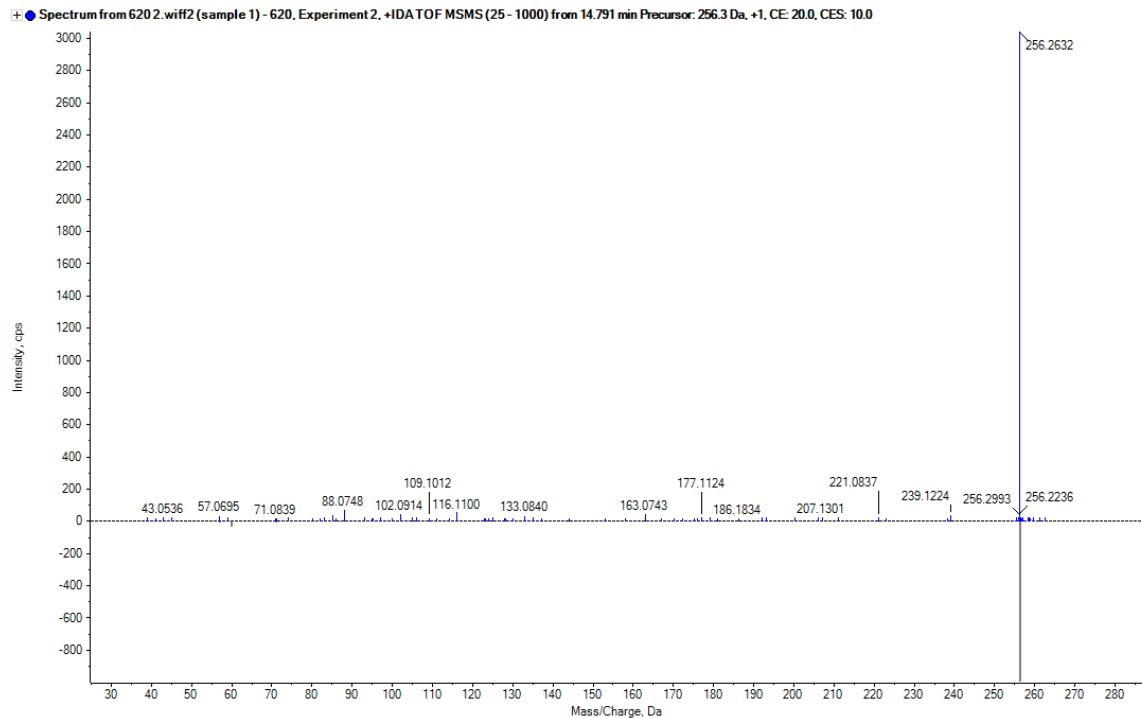


Precursor ion mass spectrum



# Compound C

## Experimental MS/MS Data

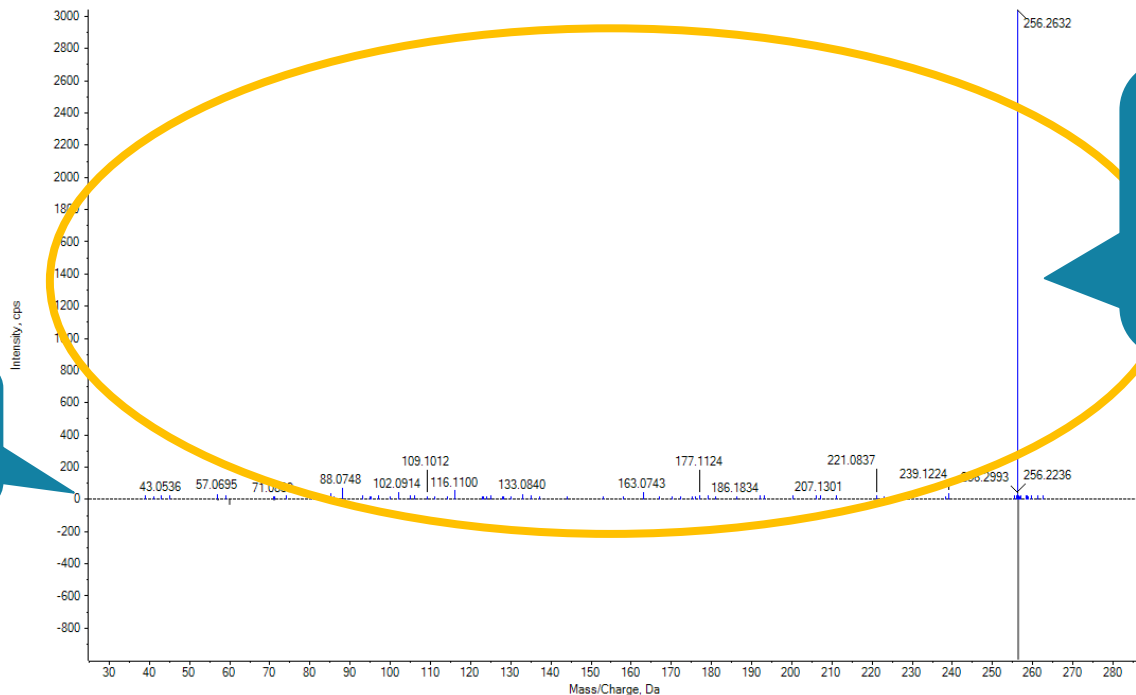


MS/MS Spectrum



# Compound C

• Spectrum from 6202.wiff2 (sample 1) - 620, Experiment 2, +IDA TOF MSMS (25 - 1000) from 14.791 min Precursor: 256.3 Da, +1, CE: 20.0, CES: 10.0



Poor library matching

MS/MS spectrum lacking diagnostic fragmentation information

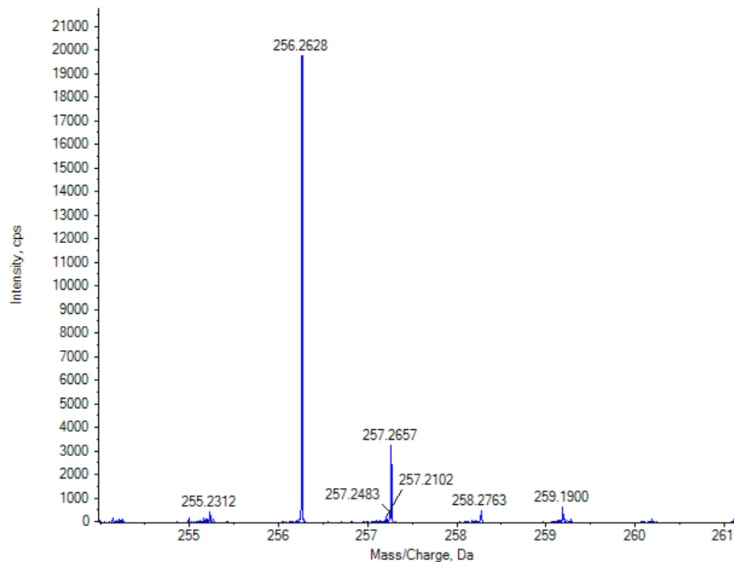
MS/MS Spectrum



# Compound C

## FORMULA FINDER AND CHEMSPIDER

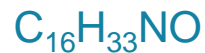
Spectrum from 620 2.wif#2 (sample 1) - 620, Experiment 1, +IDA TOF MS (100 - 2000) from 14.751 to 14.788 min



▲ Formula Finder Results

Name	Formula	Score	m/z (Da)	Error (ppm)	Error MSMS (ppm)	Hit Count
↖	C <sub>16</sub> H <sub>33</sub> NO	78.1	256.26349	2.6	1.4	3331

# Compound C



ChemSpider results for: **C16H33NO**

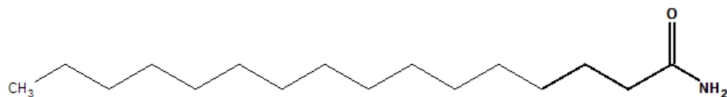
1-40 of 3331

CSID	Common Name	Molecular Weight
62629	Palmitamide	255.4393
17736	N,N-Diethyldodecanamide	255.4393
66404	N-Laurylmorpholine	255.4393
68863	MFCD00026596	255.4393
84518	N,N-Dibutyloctanamide	255.4393
81853	N,N-Dipropyldodecanamide	255.4393
3499401	MFCD00442362	255.43932

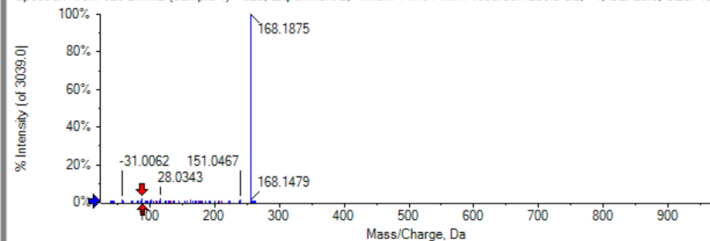
Display all Carbon Atoms

Options...

selected composition:  $C_{16}H_{33}NO^+$  (256.2632 Da)



Spectrum from 620 2.wiff2 (sample 1) - 620, Experiment 2, +...rom 14.791 min Precursor: 256.3 Da, +1, CE: 20.0, CES: 10.0



Options...

Fragments Peaks

Mass/Charge	Intensity (%)	Assigned	Error (Da)
256.2632	100.00	<input checked="" type="checkbox"/>	0.000
88.0748	2.30	<input checked="" type="checkbox"/>	0.001
116.1100	1.74	<input checked="" type="checkbox"/>	0.003
256.2236	1.61	<input checked="" type="checkbox"/>	0.040
163.0743	1.48	<input type="checkbox"/>	
102.0914	1.38	<input checked="" type="checkbox"/>	0.000
256.2993	1.25	<input checked="" type="checkbox"/>	0.036
239.1224	1.22	<input checked="" type="checkbox"/>	0.115
57.0695	1.15	<input checked="" type="checkbox"/>	0.000
85.1007	1.15	<input checked="" type="checkbox"/>	0.001
133.0840	1.12	<input type="checkbox"/>	

Matches: 20 of 26 peaks, 95.8% of total intensity



# Compound C

## CHEMSPIDER MATCHES

ChemSpider results for: C<sub>16</sub>H<sub>33</sub>NO

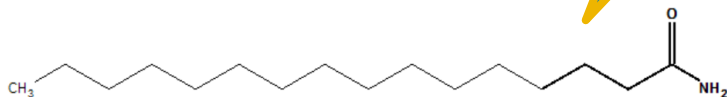
1-40 of 3331

CSID	Common Name
62629	Palmitamide
17736	N,N-Diethyldodecanamide
66404	N-Laurylmorpholine
68863	MFCD00026596
84518	N,N-Dibutyloctanamide
81853	N,N-Dipropyldodecanamide
3499401	MFCD00442362

Display all Carbon Atoms

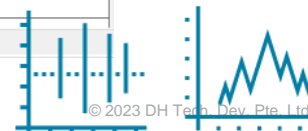
selected composition: C<sub>16</sub>H<sub>33</sub>NO<sup>+</sup> (88.0757 Da)

Palmitamide is used as an additive in tires and asphalt



Mass/Charge	Intensity (%)	Assigned	Error (Da)
256.2632	100.00	<input checked="" type="checkbox"/>	0.000
88.0748	2.30	<input checked="" type="checkbox"/>	0.001
116.1100	1.74	<input checked="" type="checkbox"/>	0.003
256.2236	1.61	<input checked="" type="checkbox"/>	0.040
163.0743	1.48	<input type="checkbox"/>	
102.0914	1.38	<input checked="" type="checkbox"/>	0.000
256.2993	1.25	<input checked="" type="checkbox"/>	0.036
239.1224	1.22	<input checked="" type="checkbox"/>	0.115
57.0695	1.15	<input checked="" type="checkbox"/>	0.000
85.1007	1.15	<input checked="" type="checkbox"/>	0.001
133.0840	1.12	<input type="checkbox"/>	

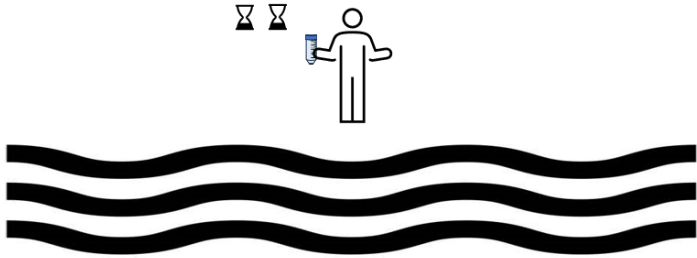
Matches: 20 of 26 peaks, 95.8% of total intensity





# Summary

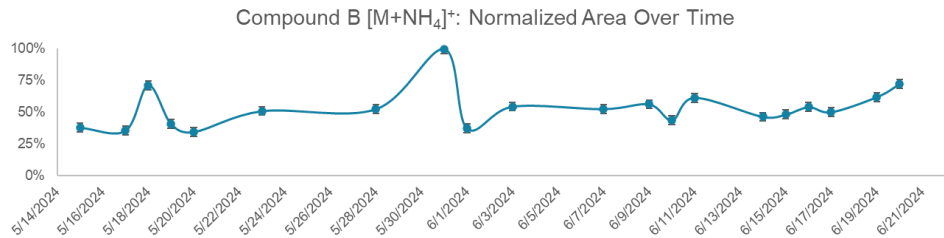
## Spatio-temporal Monitoring and HRMS





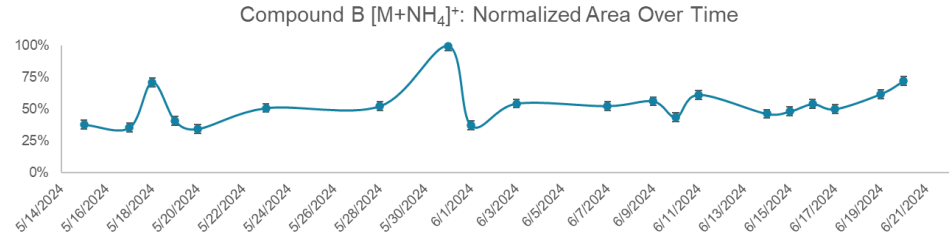
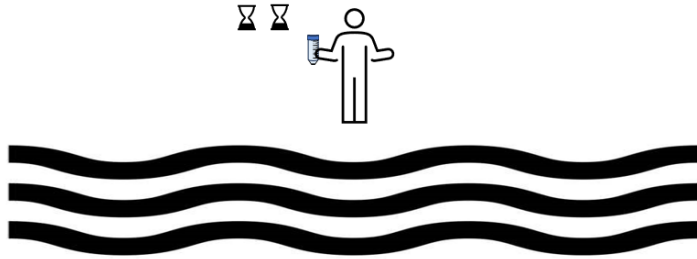
# Summary

## Spatio-temporal Monitoring And HRMS

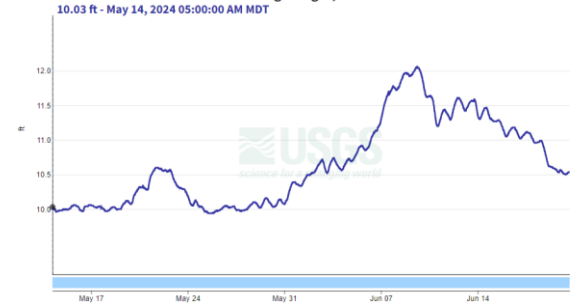


# Summary

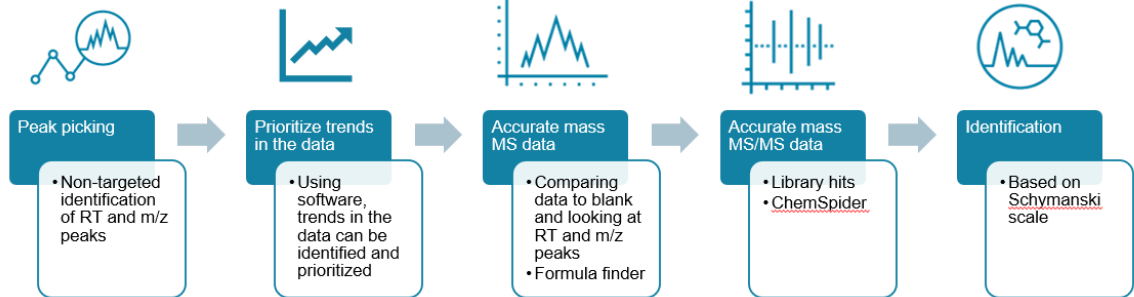
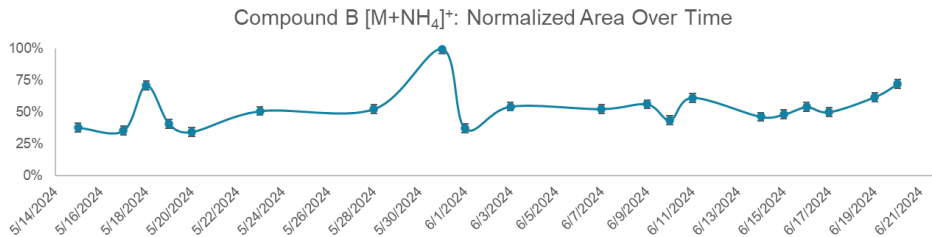
## Spatio-temporal Monitoring And HRMS



**ST Vrain CR Blw Boulder CR at Hwy 119 NR Longmont - 06730525**  
August 6, 2023 - August 5, 2024  
Gage height, feet



## Spatio-temporal Monitoring And HRMS



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Gage height, feet



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