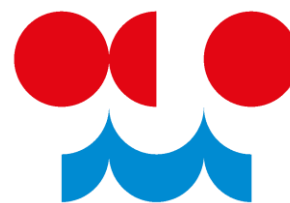




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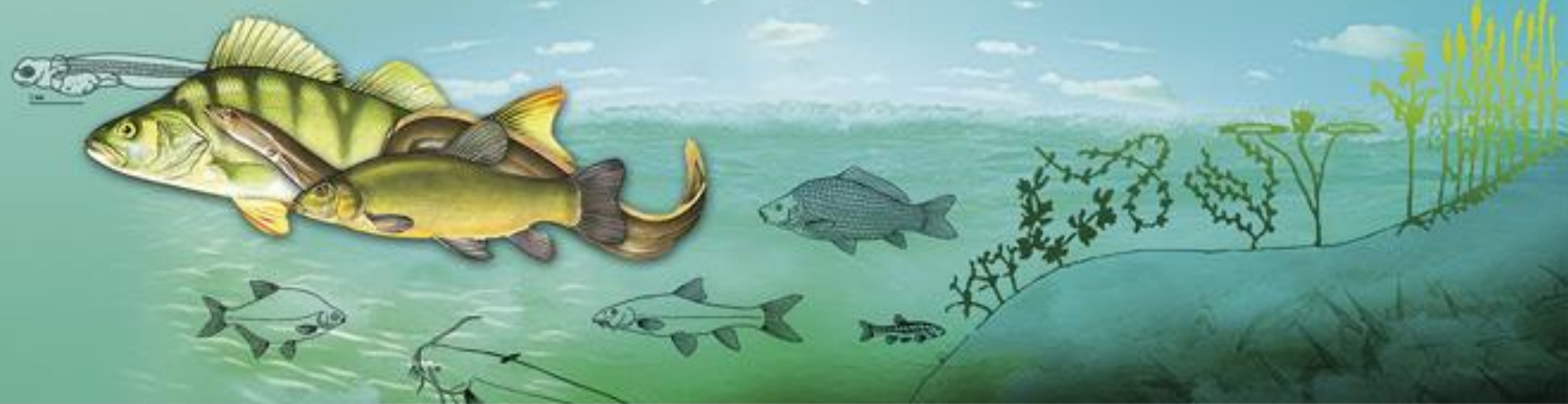


ČESKÝ
HYDROMETEOROLOGICKÝ
ÚSTAV

COWI



How can we exploit non-targeted screening data from passive samplers?



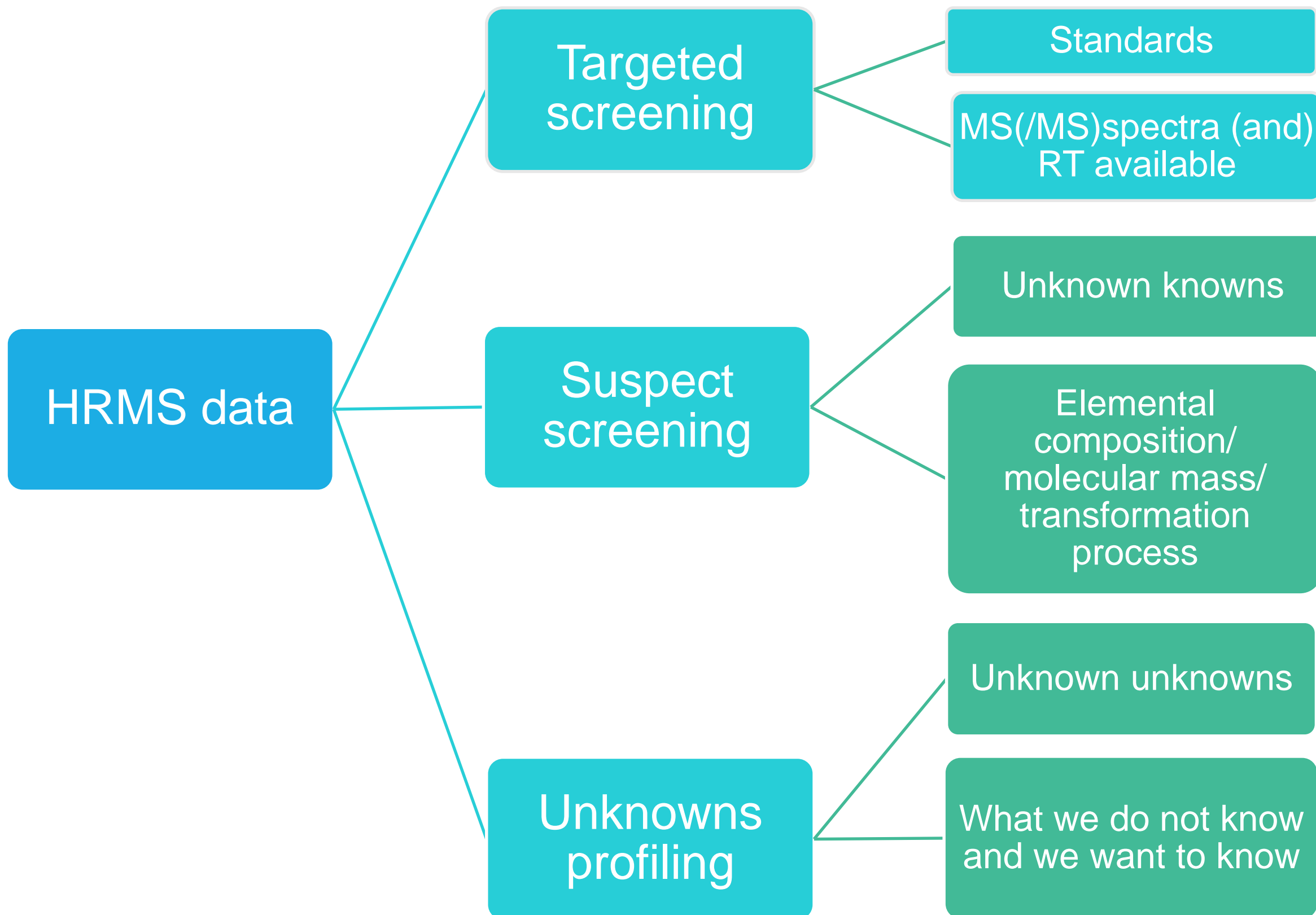
Grabic R.

Kodeš V., Bergqvist P.A., Dalen H., Grabicová K., Vojs
Staňová A., Bořík A., Švecová H., Randák T.

www.frov.jcu.cz



What is the unknown screening?





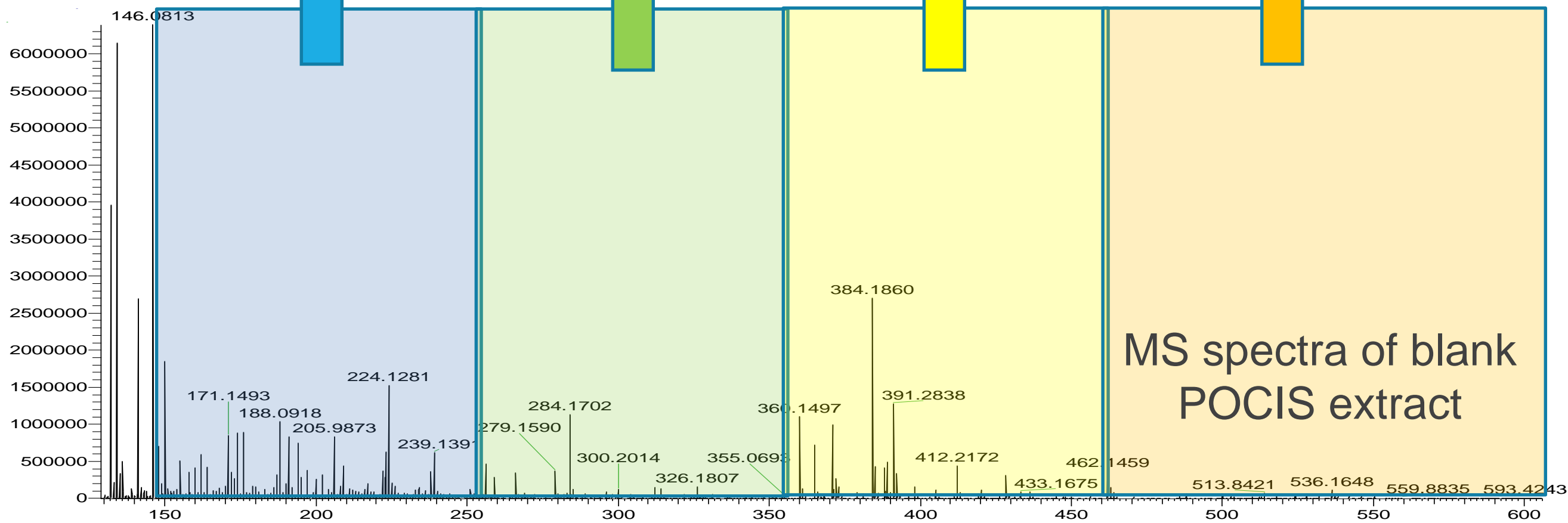
HRPS – high resolution product scan – 17500 FWHM



Collision – stepped CID to achieve fragmentation for as many as possible compounds



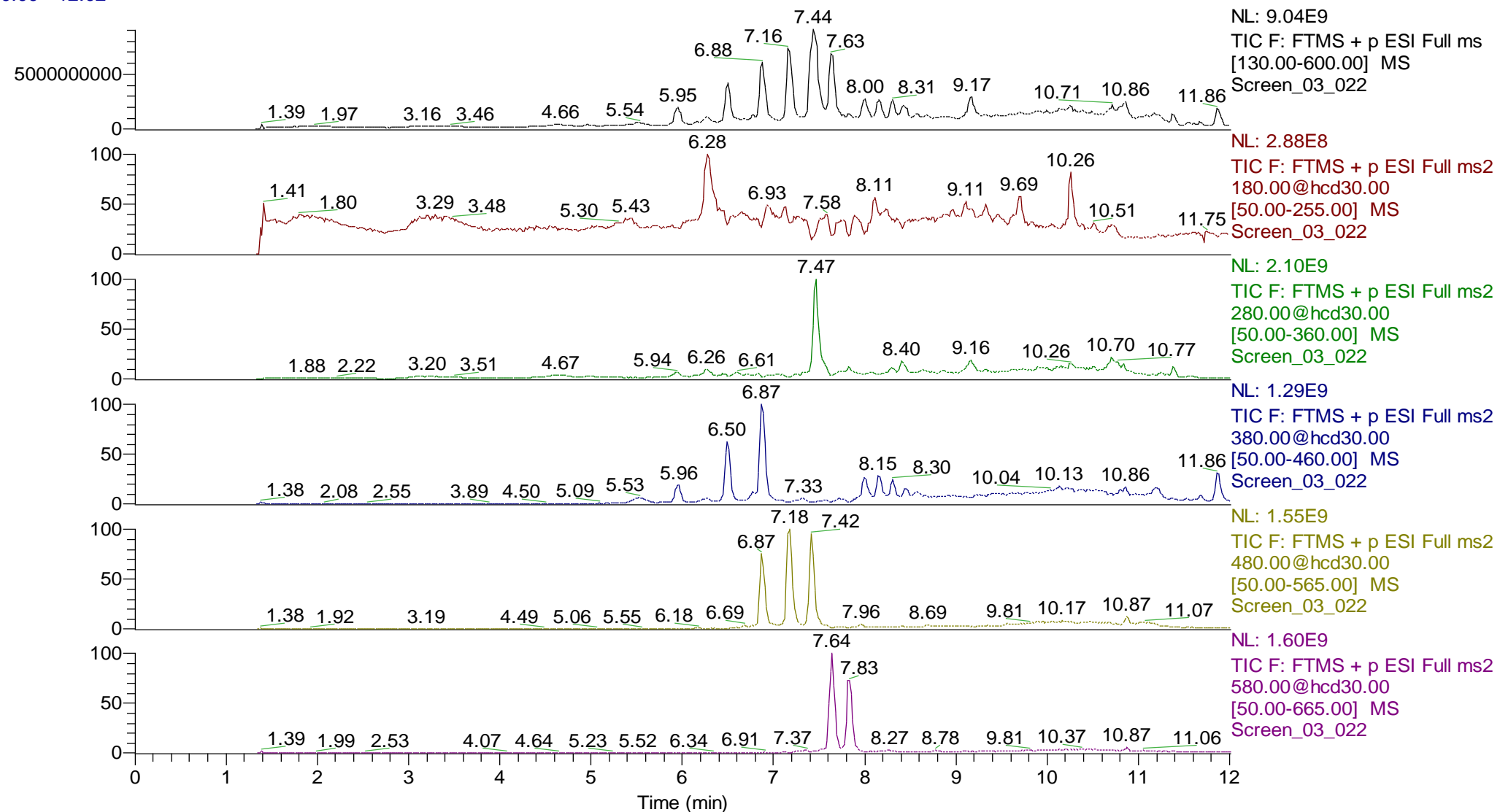
Isolation – filling orbital trap (AGC set up of ion population and filling time)

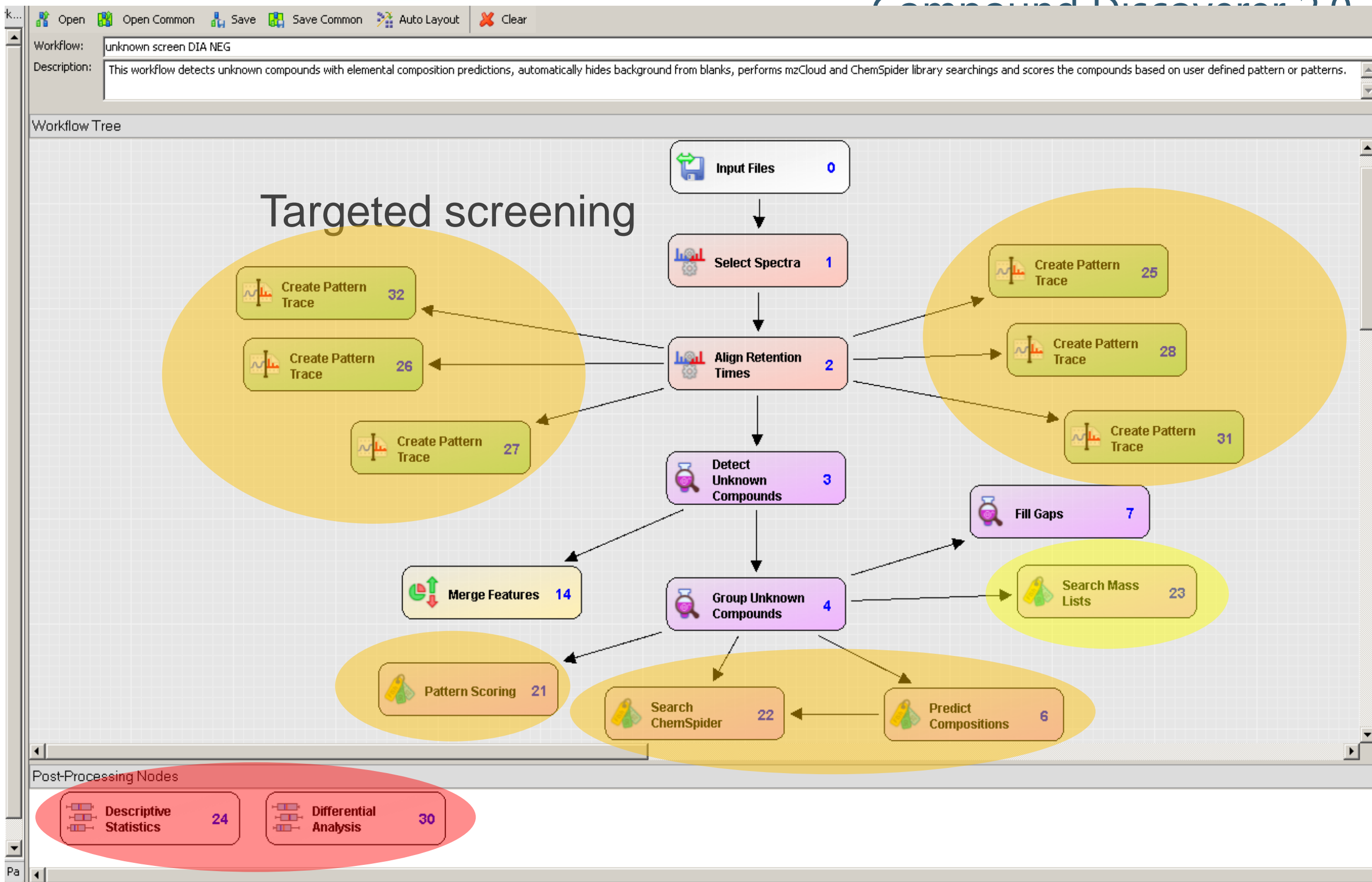




- ❖ Standardized LC-HRMS/DIA method – hybrid quadrupole/ orbital trap mass spectrometer QExactive
- ❖ EVO C18 column 50 x 2.1 x 3 µm particles
- ❖ Water/MeOH buffered with 10 mmol NH₄Ac and 0.1 % FA
- ❖ One analysis in pos and one in neg ESI

RT: 0.00 - 12.02



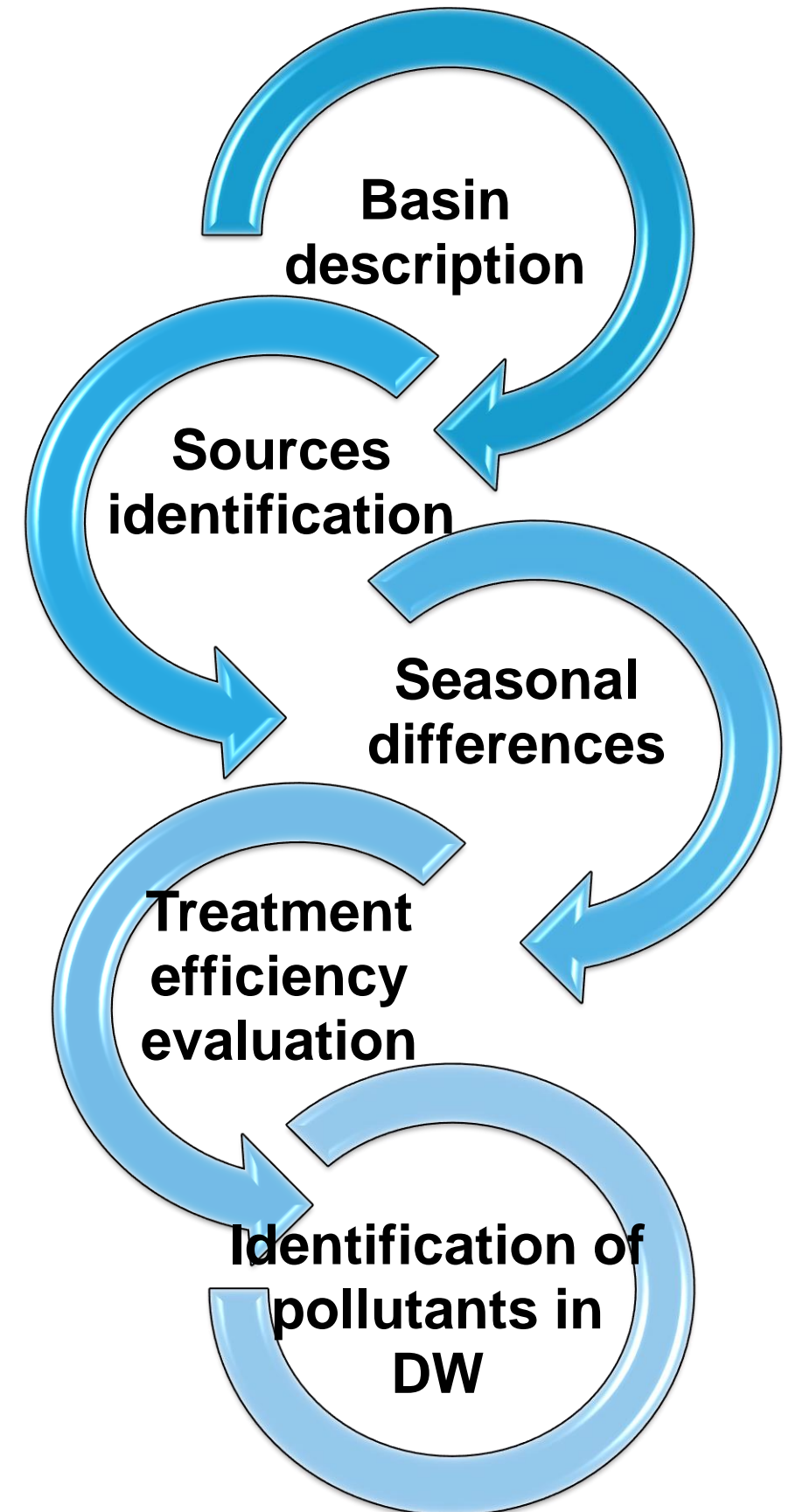
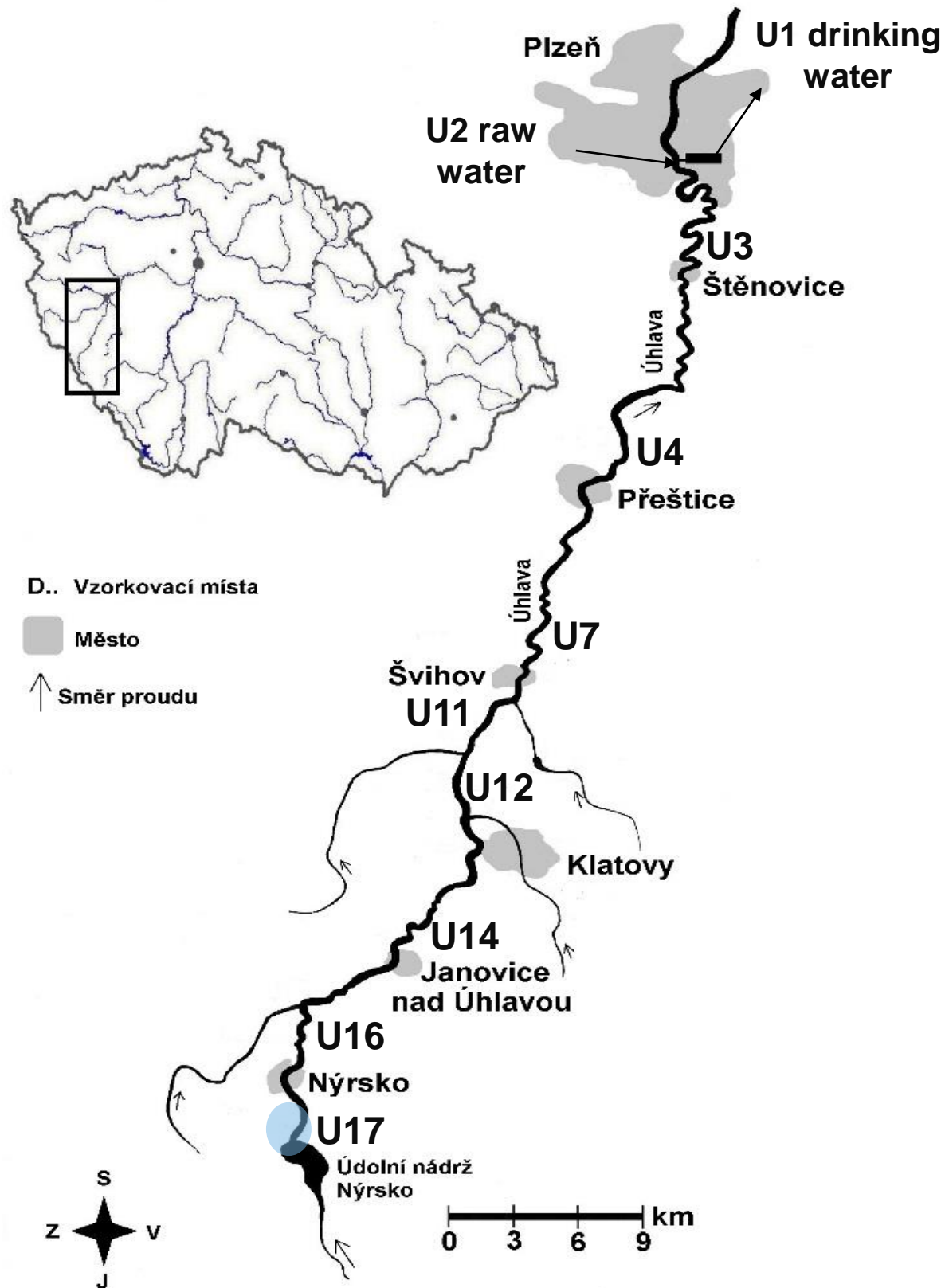




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Example 1 case study on drinking water treatment plant

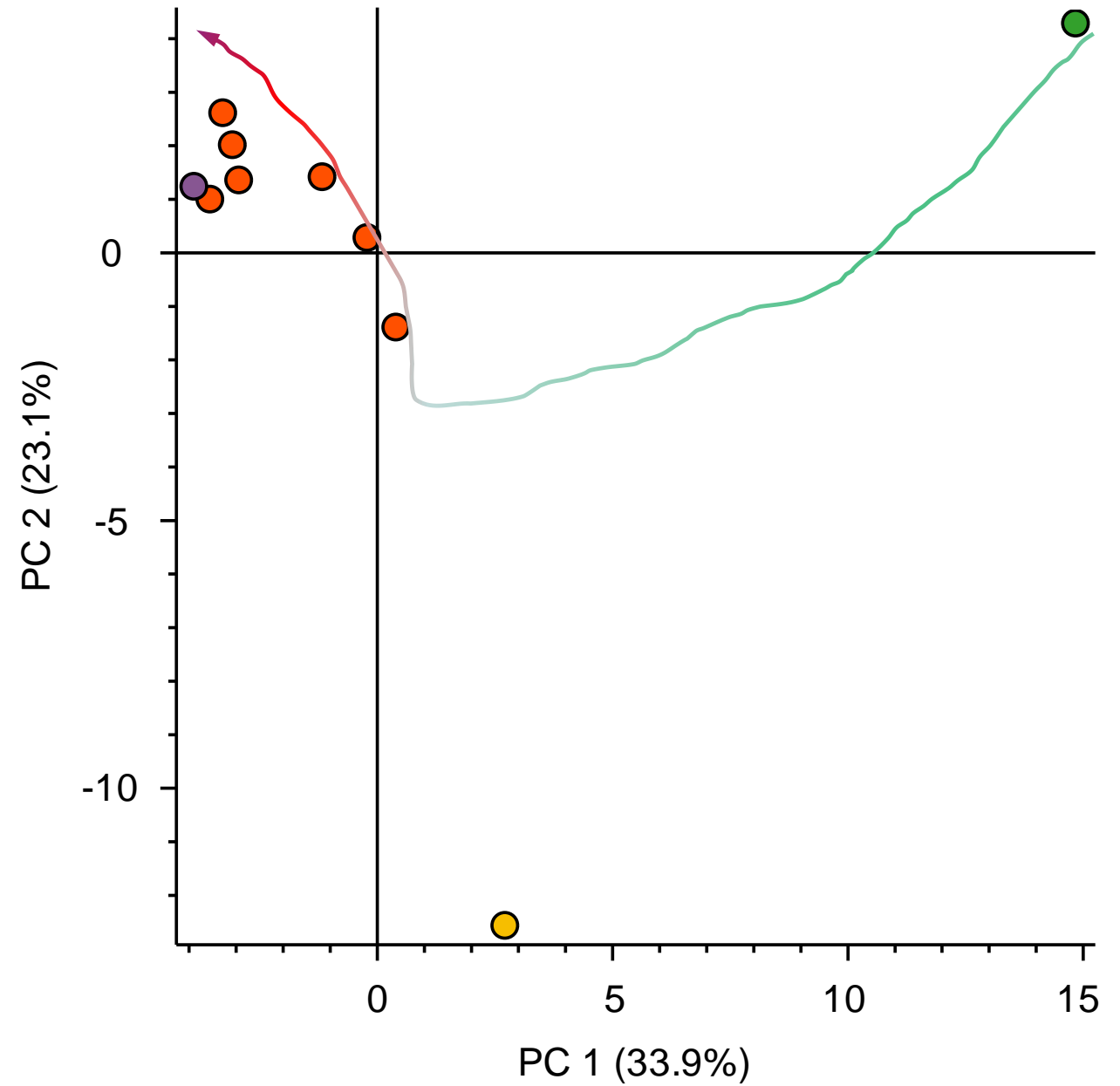
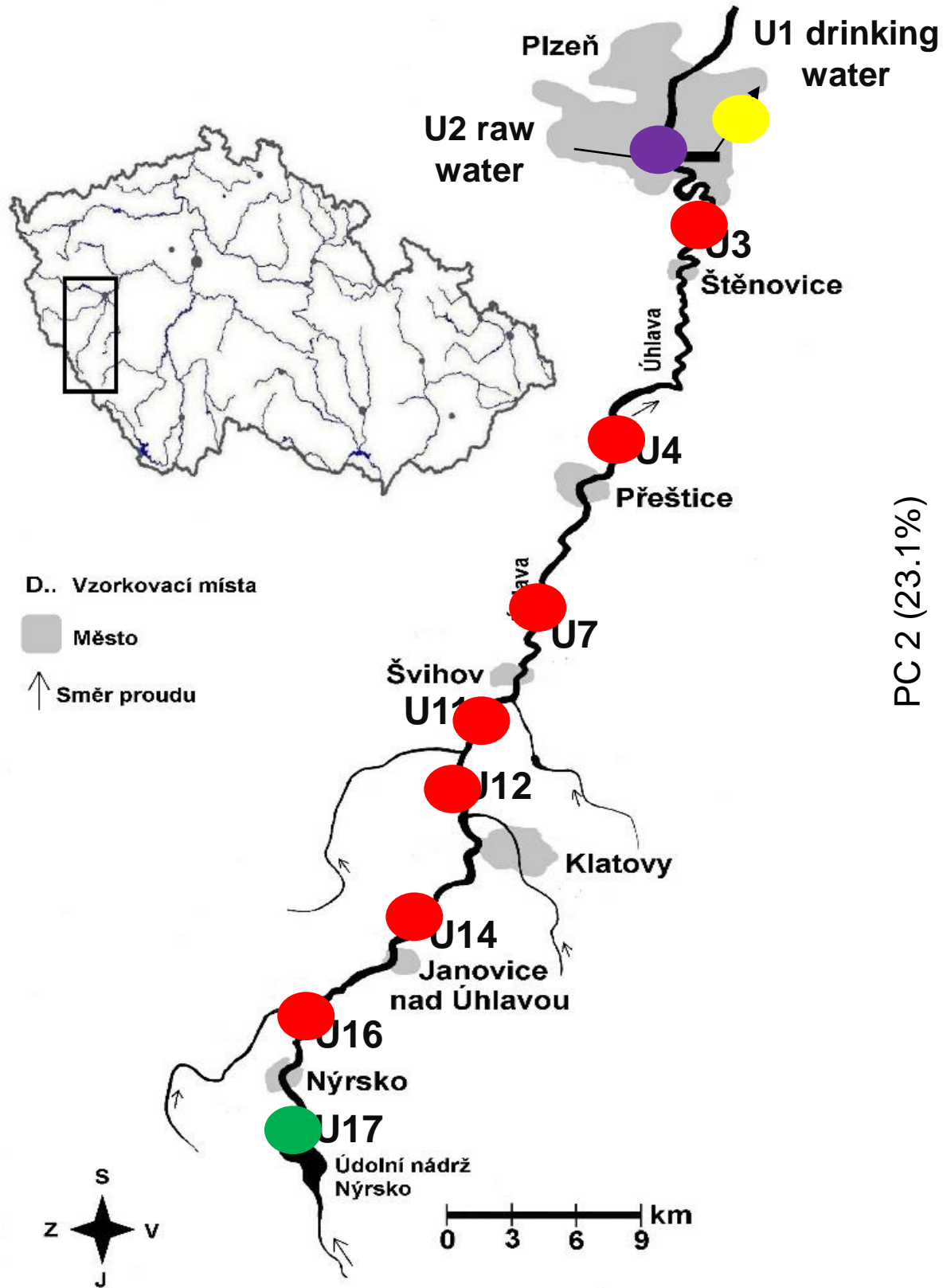




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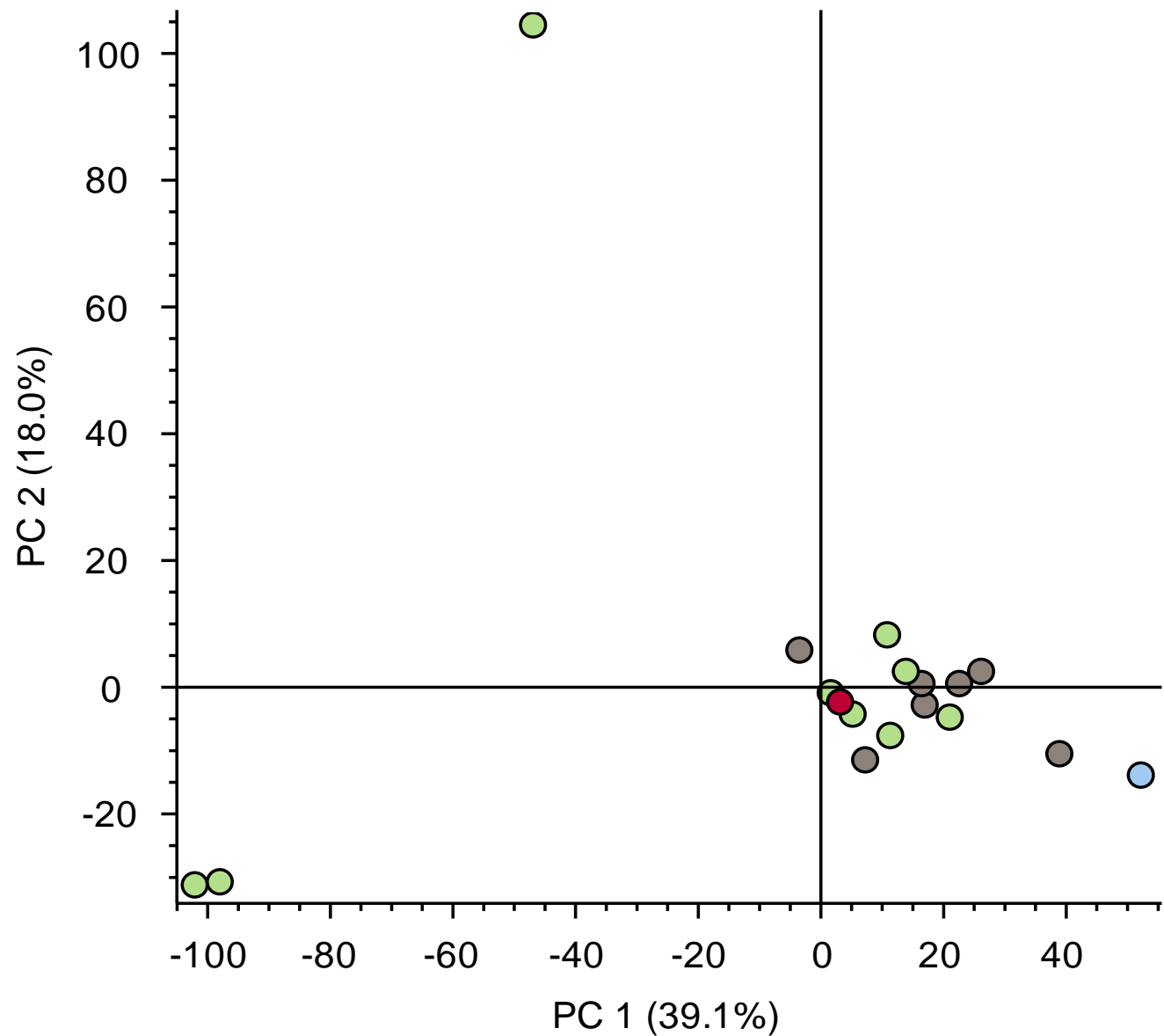
Example 1 case study on drinking water treatment plant





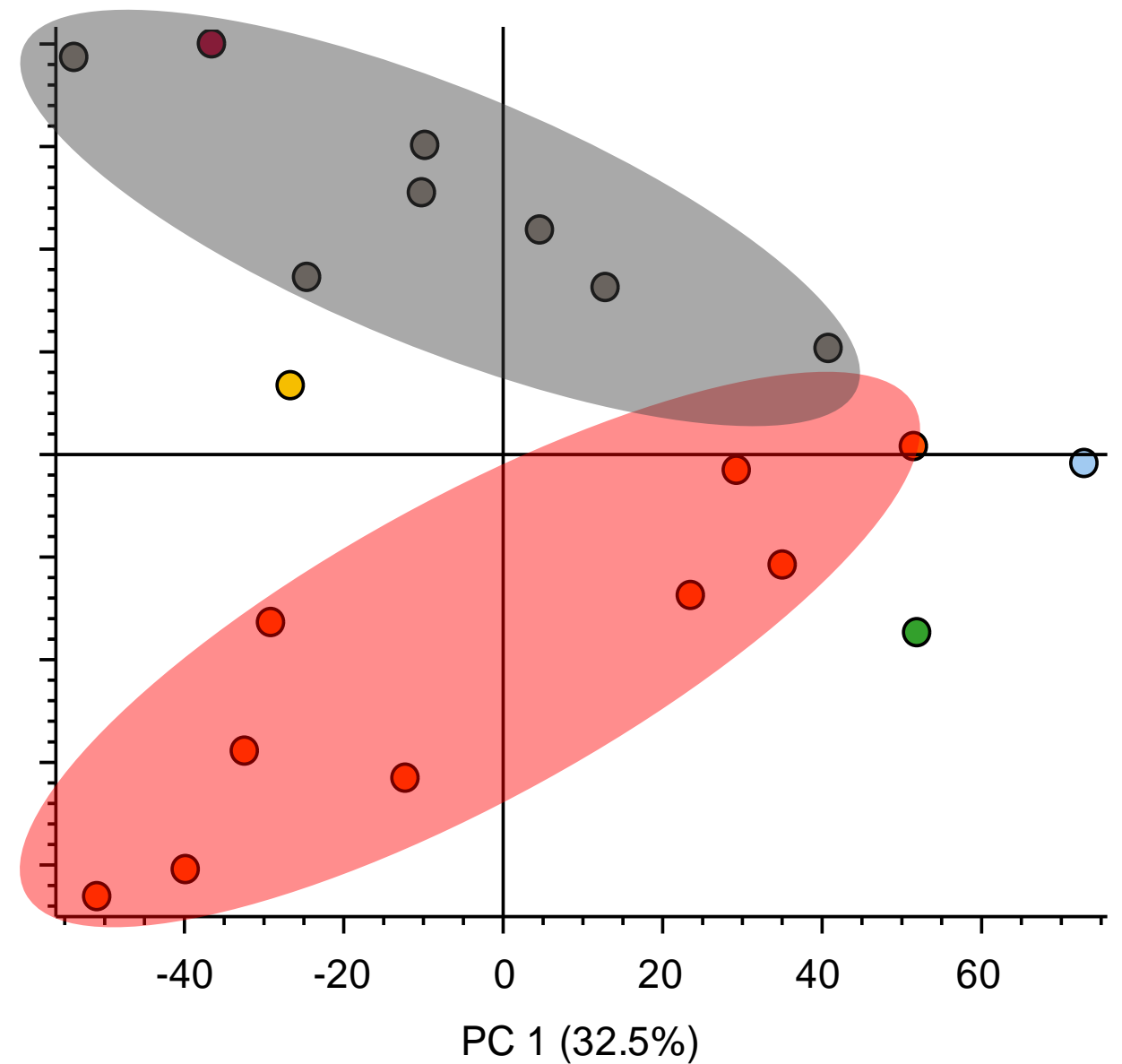
Example 1 case study on drinking water treatment plant

Identification of pollution sources



- warm, drinking, Sample
- warm, raw, Sample
- warm, tributaries, Sample
- warm, Uhlava, Sample

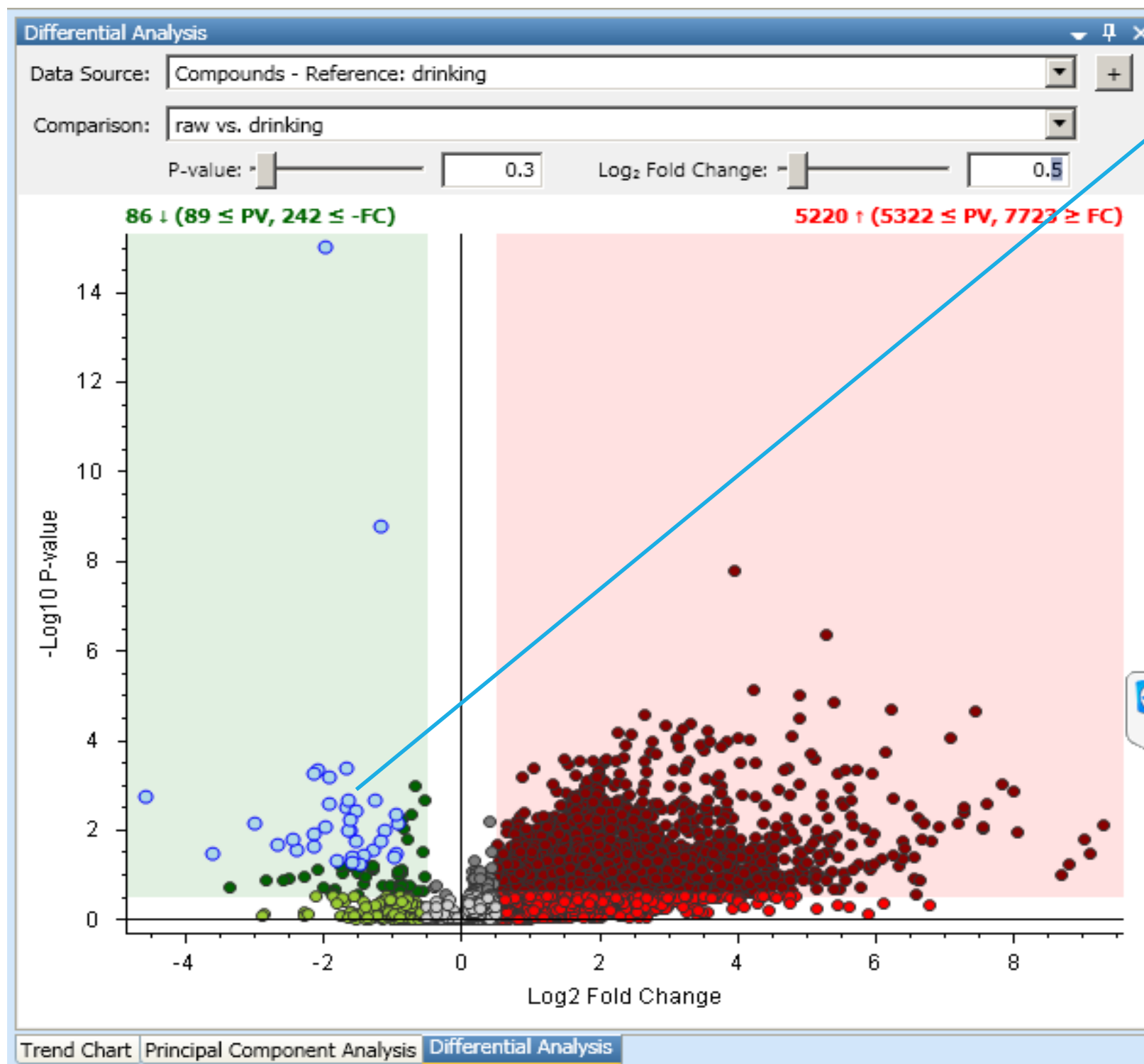
Seasonal variations



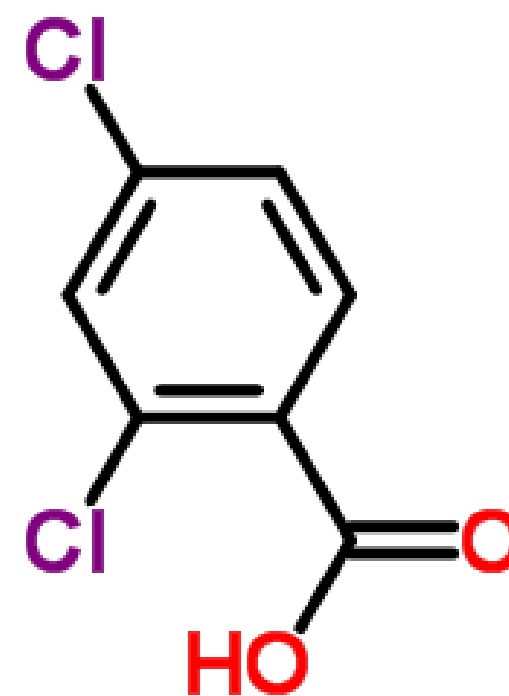
- cold, drinking, Sample
- cold, raw, Sample
- cold, Uhlava, Sample
- warm, drinking, Sample
- warm, raw, Sample
- warm, Uhlava, Sample



Example 1 case study on drinking water treatment plant

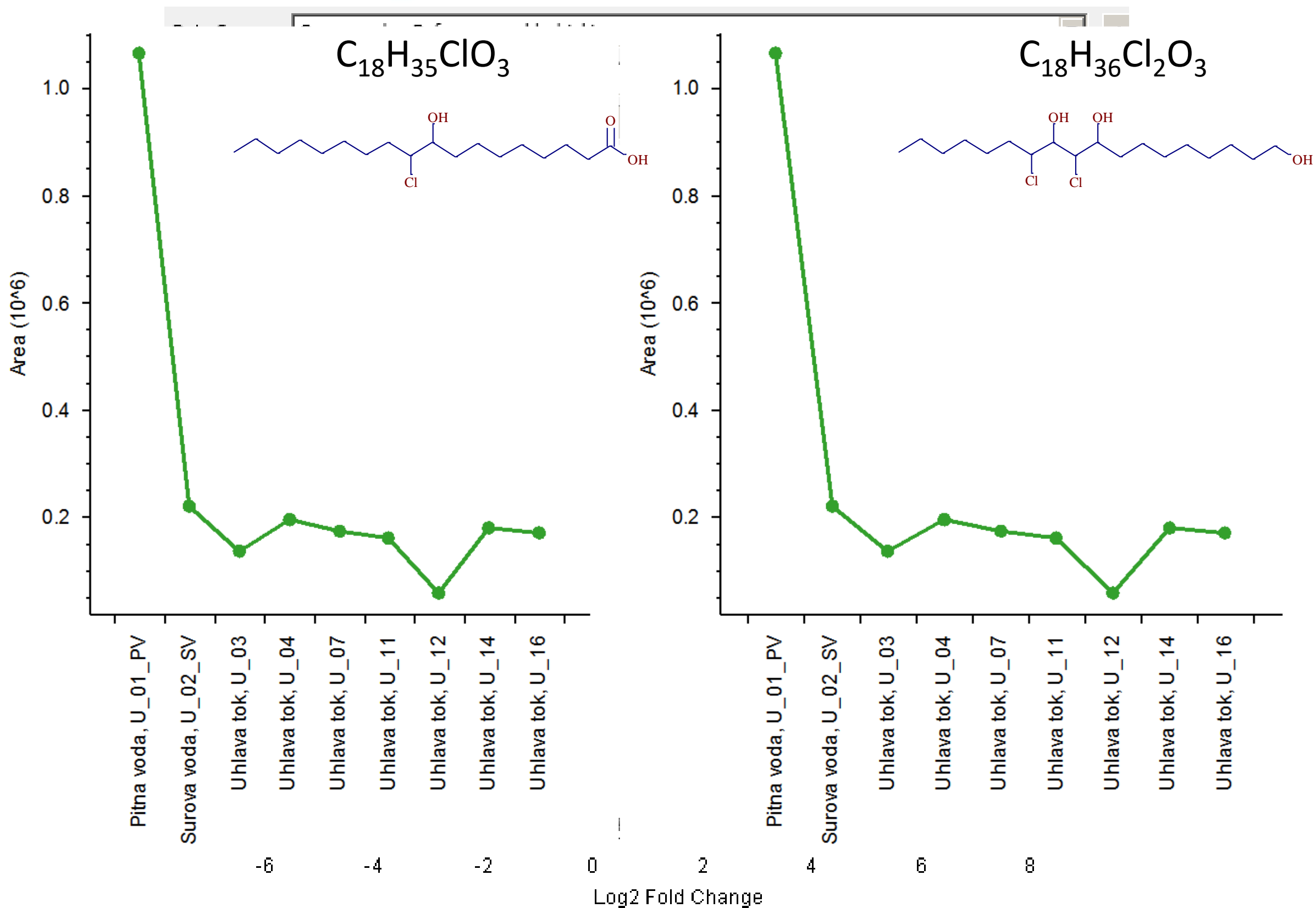


Chempider results - 8 hits
all of them izomers





Example 1 case study on drinking water treatment plant





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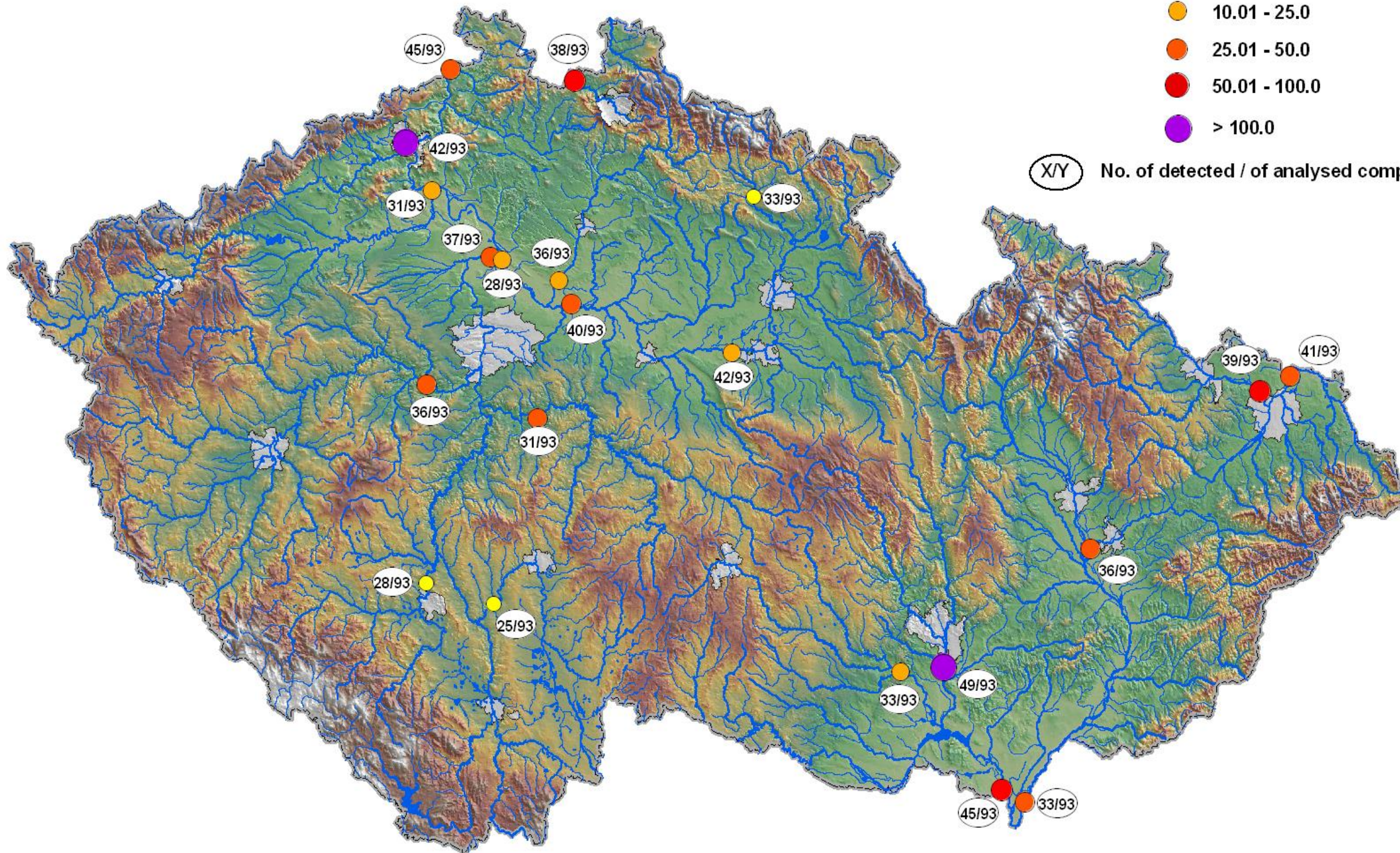
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Czech Republic

Example 2 CHMI annual surface water quality monitoring

Total concentration [ng/POCIS/day]

- < 5.00
- 5.01 - 10.00
- 10.01 - 25.0
- 25.01 - 50.0
- 50.01 - 100.0
- > 100.0

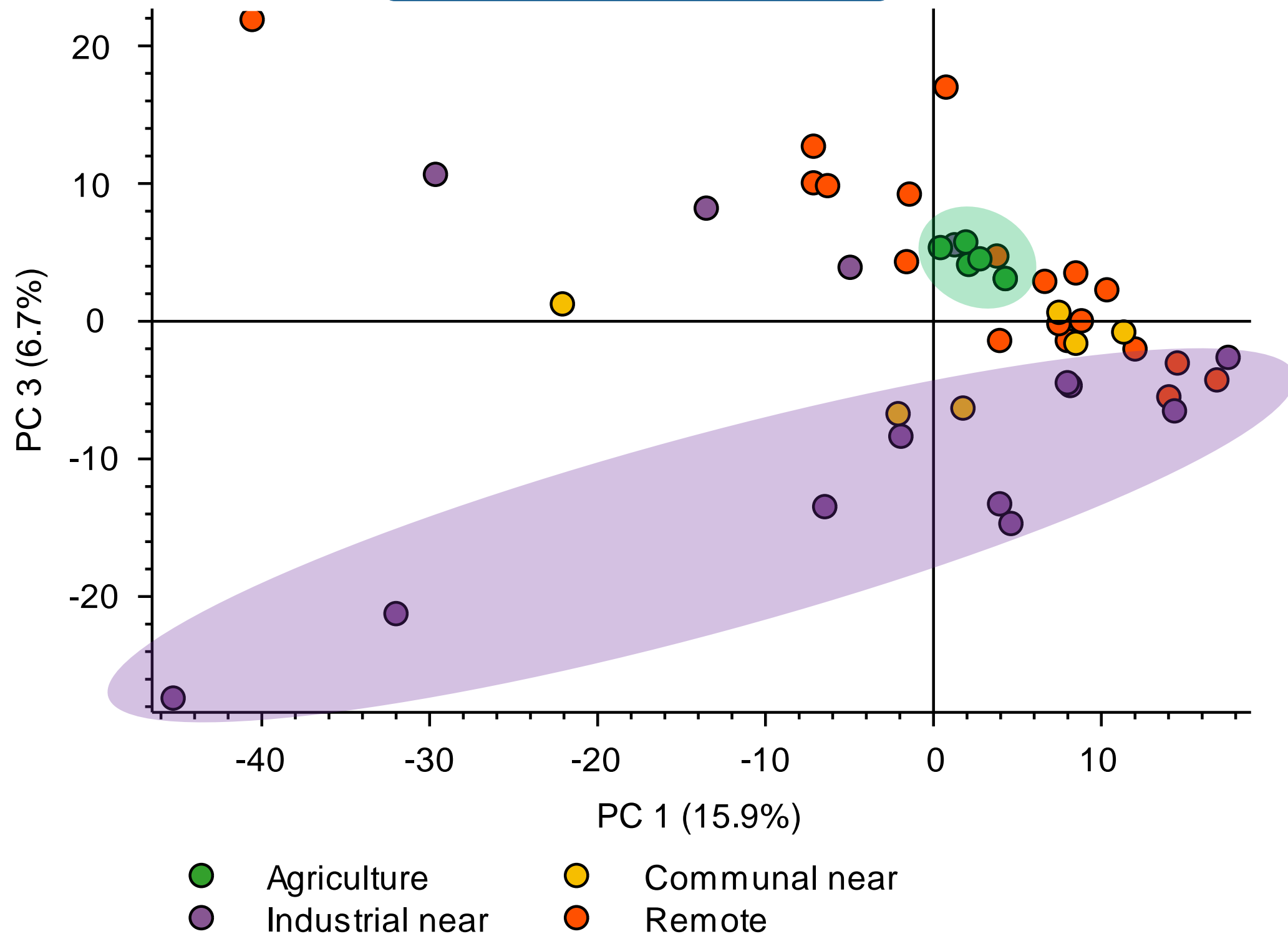
(X/Y) No. of detected / of analysed compounds





Example 2 CHMI annual surface water quality monitoring

Grouping by source





Example 2 CHMI annual surface water quality monitoring

Compound Discoverer 2.0.0.303
Reporting Libraries View Help

Start Page **CHMI_neg_new01** CHMI_2017neg*

Chromatograms

Group By:
 Season (3/3)
 Basins (6/6)
 Source (5/5)
 Sample Type (2/2)
 Sample (46/46)

Filter By:
 Season
 Basins
 Source
 Sample Type
 Sample

Source: Agriculture
Sample Type: Sample
Source: Industrial near
Sample Type: Sample
Source: Remote
Sample Type: Sample
Source: Communal near
Sample Type: Sample
Source: n/a
Sample Type: Blank

Intensity [counts] (10⁶)

RT [min]

Mass Spectrum
#3295, RT=8.574 min, FTMS (-)
#3297, RT=8.580 min, FTMS (-)

Filters Chromatograms

Compounds Compounds per File Merged Features Features Custom Explanations ChemSpider Results Mass List Search Results Specialized Traces

Checked	Name	Predicted Formula	Molecular Weight	RT [min]	Area (Max.)	# ChemSpider Results	Mass List Matches	Pattern Matches
<input checked="" type="checkbox"/>		C12 H11 F3 N2 O3	288.07244	8.590	9807392	5		
<input checked="" type="checkbox"/>		C12 H26 O6 S	298.14522	10.048	5233855	2		
<input checked="" type="checkbox"/>		C13 H13 F2 N6 O5 P	402.06532	8.588	2822164	7		
<input checked="" type="checkbox"/>		C7 H7 Cl O4 S	221.97559	7.680	2096765	4		
<input checked="" type="checkbox"/>		C6 H4 Cl2 O4 S	241.92105	8.216	1843530	3		
<input checked="" type="checkbox"/>		C13 H10 O6 S	294.01996	8.607	1794131	2		
<input checked="" type="checkbox"/>		C15 H19 F2 O3 P	316.10403	9.710	1525618	12		
<input checked="" type="checkbox"/>		C11 H9 F3 N2 O2	258.06205	8.901	1484630	11		
<input checked="" type="checkbox"/>		C26 H38 N2 O3	426.28859	10.917	1465855	5		
<input checked="" type="checkbox"/>		C10 H8 O3 S	208.01958	6.735	1356249	20		
<input checked="" type="checkbox"/>		C6 H11 N3 O12	317.03461	7.725	1150528	13		
<input checked="" type="checkbox"/>		C9 H20 O4 S	224.10850	10.033	1141100	5		
<input checked="" type="checkbox"/>		C9 H6 F N2 O2 P	224.01455	7.310	1092897	23		
<input checked="" type="checkbox"/>			213.14436	9.890	930277	2		

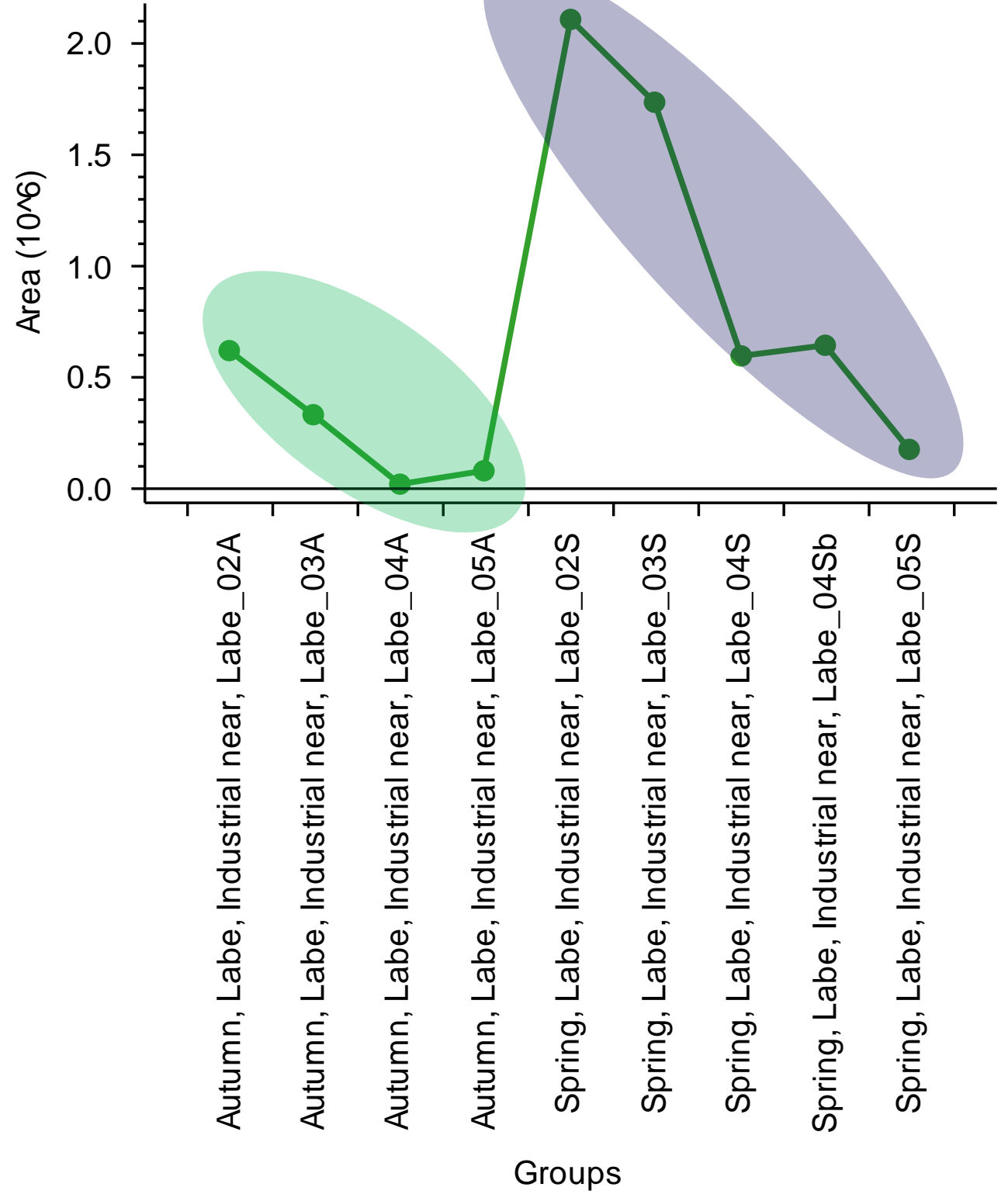
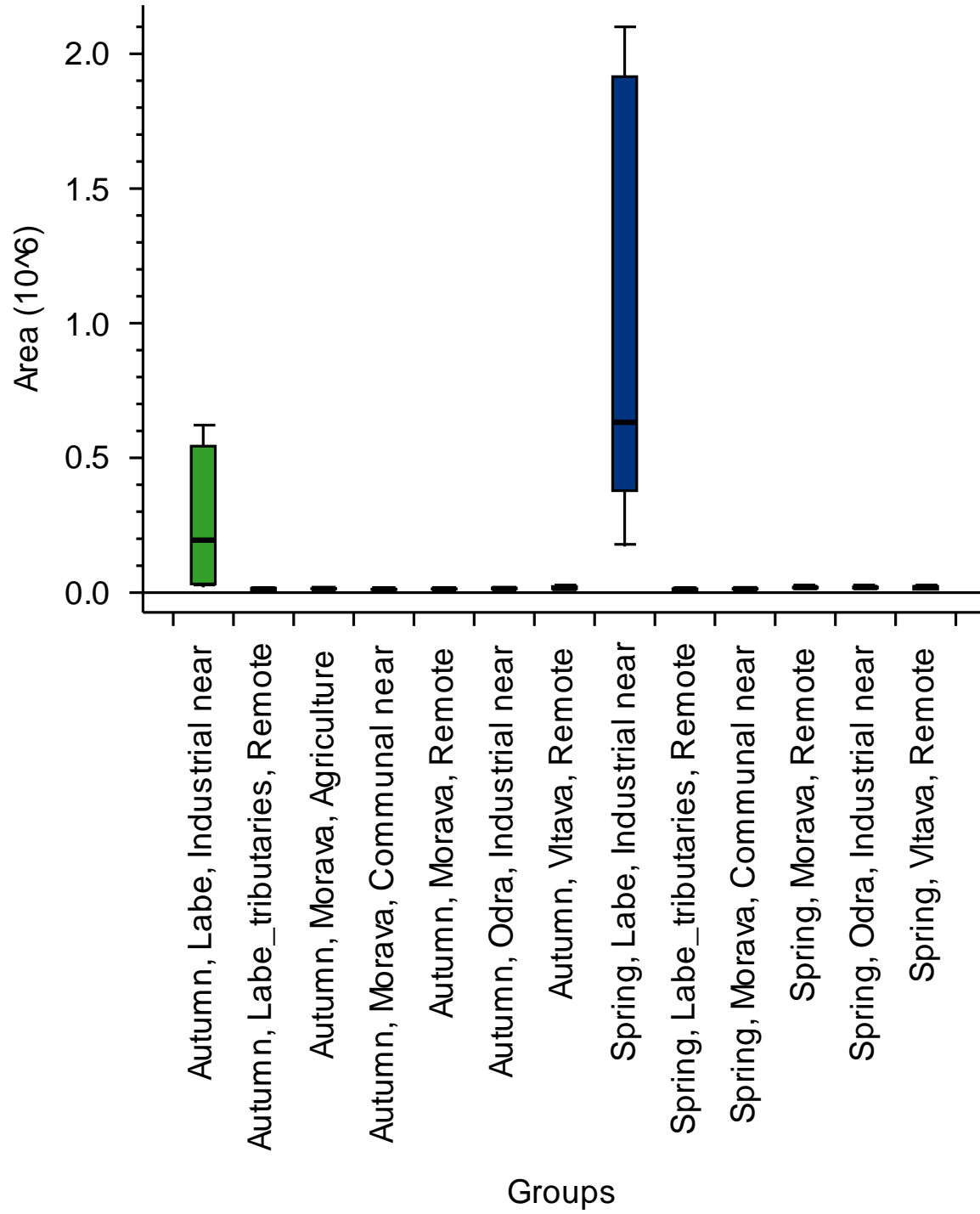
Side Related Tables

Predicted Compositions Compounds per File Matched Patterns ChemSpider Results Mass List Search Results

Checked	Formula	Molecular Weight	Is known to ChemSpider	ΔMass [Da]	ΔMass [ppm]	SFit [%]	# MI	RDBE
<input type="checkbox"/>	C12 H11 F3 N2 O3	288.07218	X	0.00026	0.91	74	3	7.0
<input type="checkbox"/>	C13 H15 F2 O3 P	288.07269		-0.00025	-0.86	60	3	6.0



Example 2 CHMI annual surface water quality monitoring



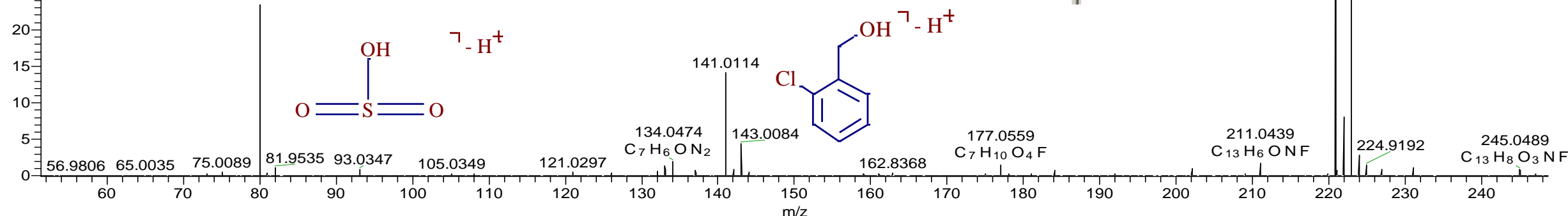
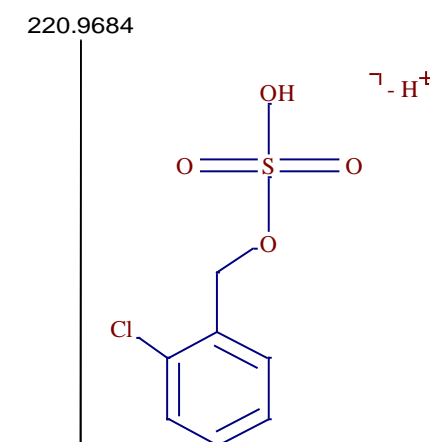
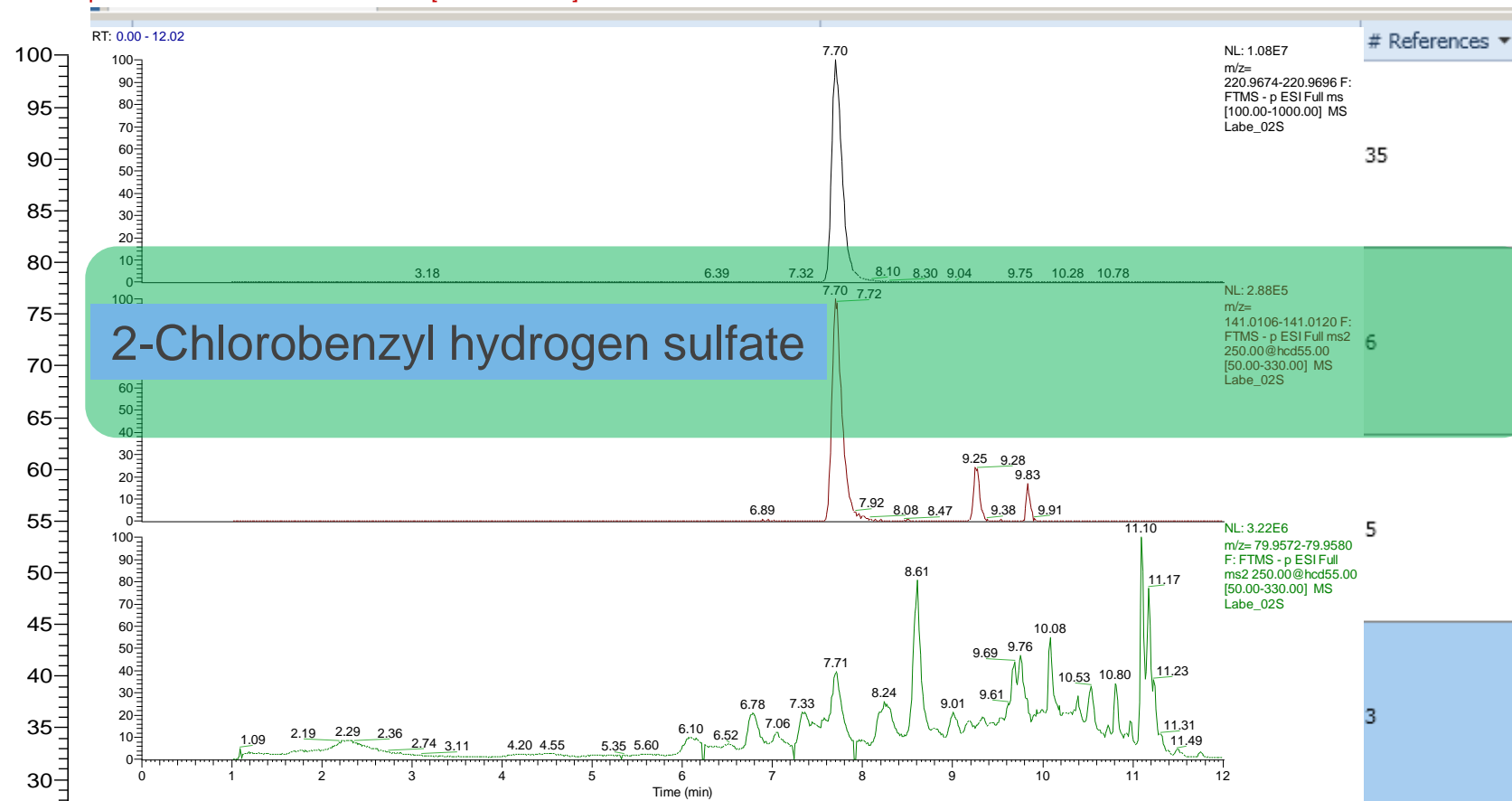


Example 2 CHMI annual surface water quality monitoring

Hide Related Tables

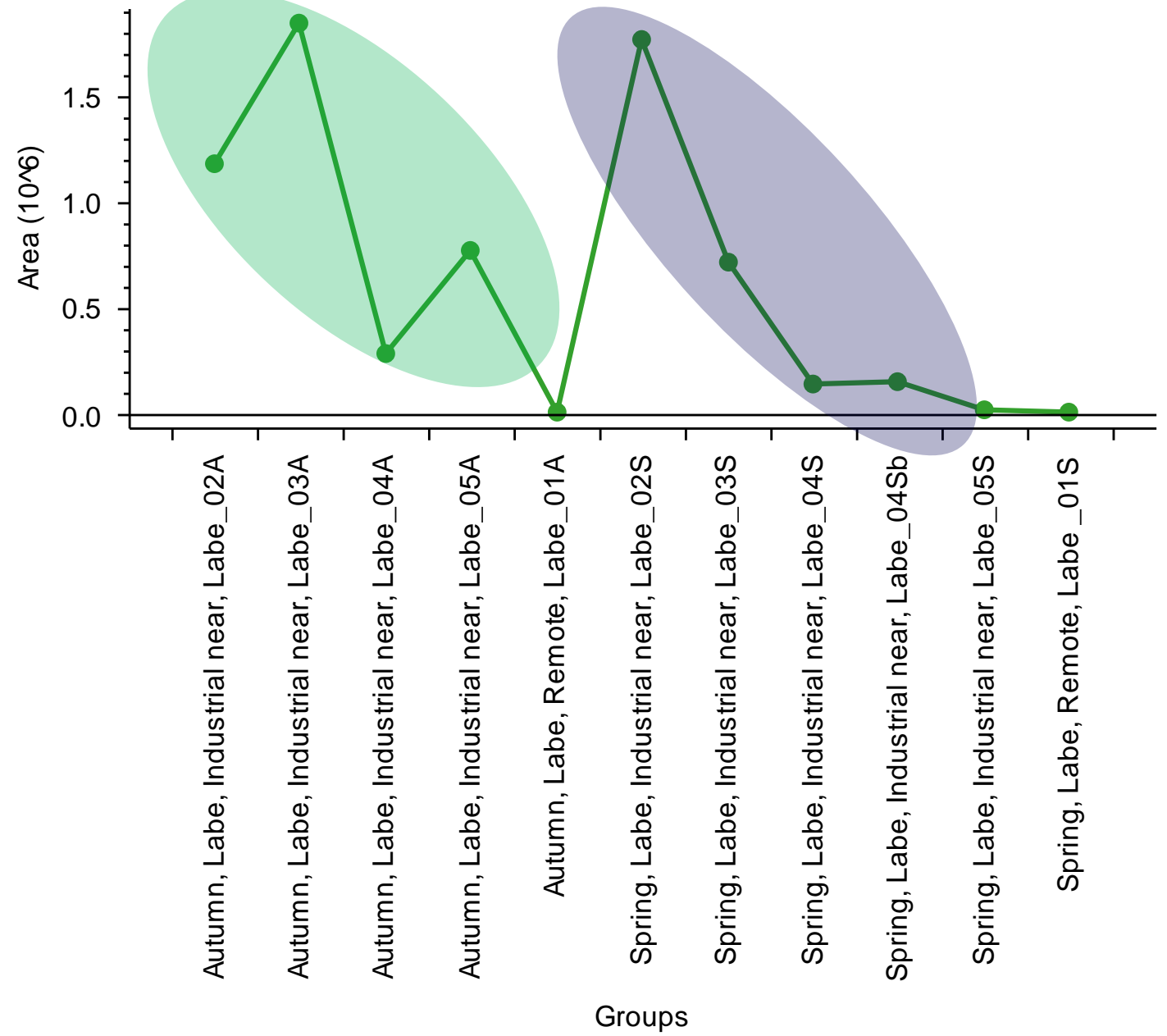
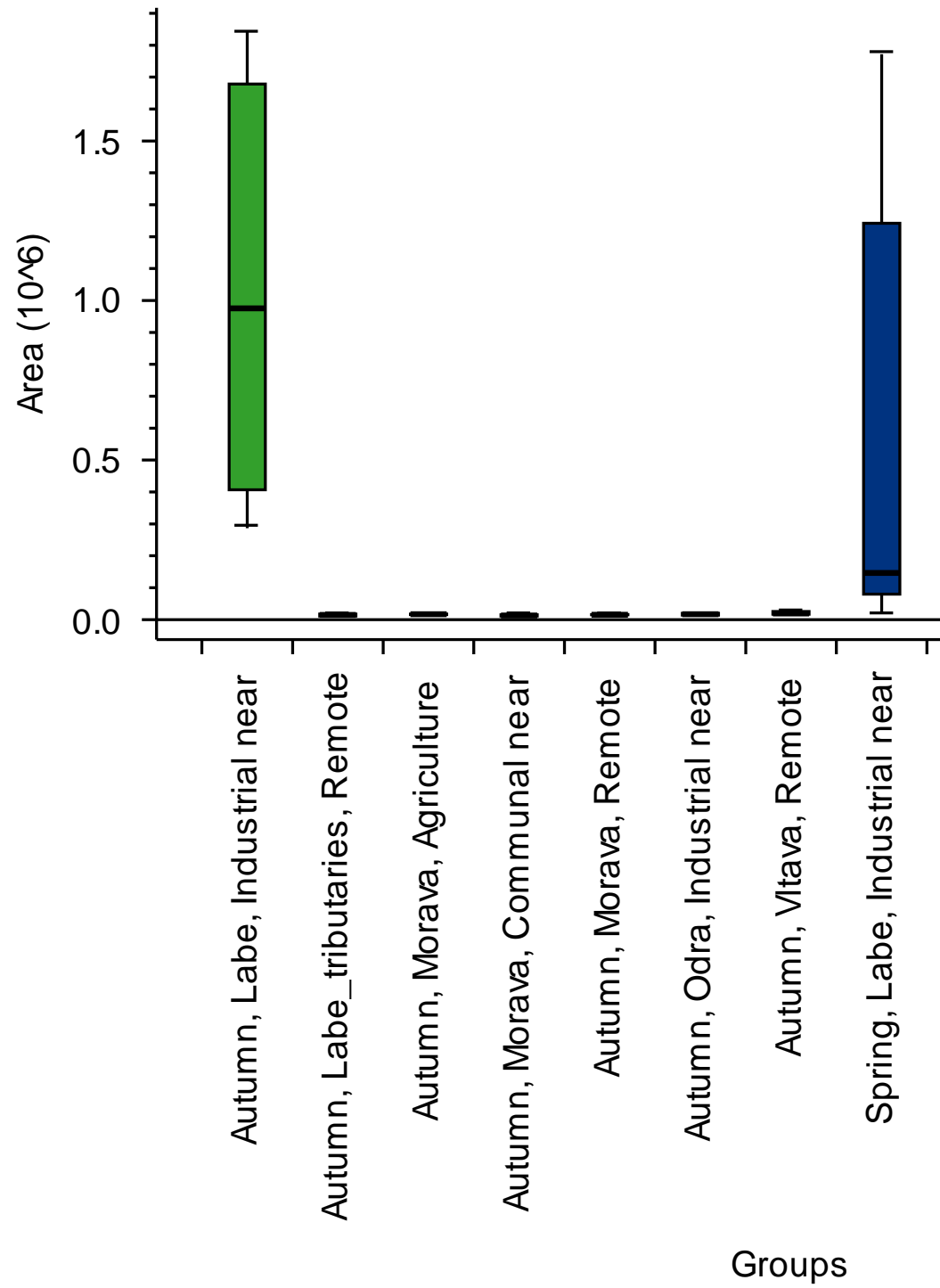
	Predicted Compositions	Compounds per File	Matched Patterns	ChemSpider Results	Mass List Search Results				
	Checked	Formula	Molecular Weight	Is known to ChemSpider	Δ Mass [Da]	Δ Mass [ppm]	SFit [%]	# MI	RDBE
1	<input type="checkbox"/>	C7 H7 Cl O4 S	221.97536	X	0.00024	1.07	70	5	4.0
2	<input type="checkbox"/>	C6 H5 Cl F N2 O2 P	221.97612		-0.00052	-2.36	68	4	5.0
3	<input type="checkbox"/>	C5 H5 F N2 O3 P2	221.97594		-0.00035	-1.57	64	2	5.0

Labe_02S #2893-2922 RT: 7.70-7.75 AV: 5 SB: 96 7.05-7.56 , 8.00-8.76 NL: 1.58E6
F: FTMS - p ESI Full ms2 250.00@hcd55.00 [50.00-330.00]



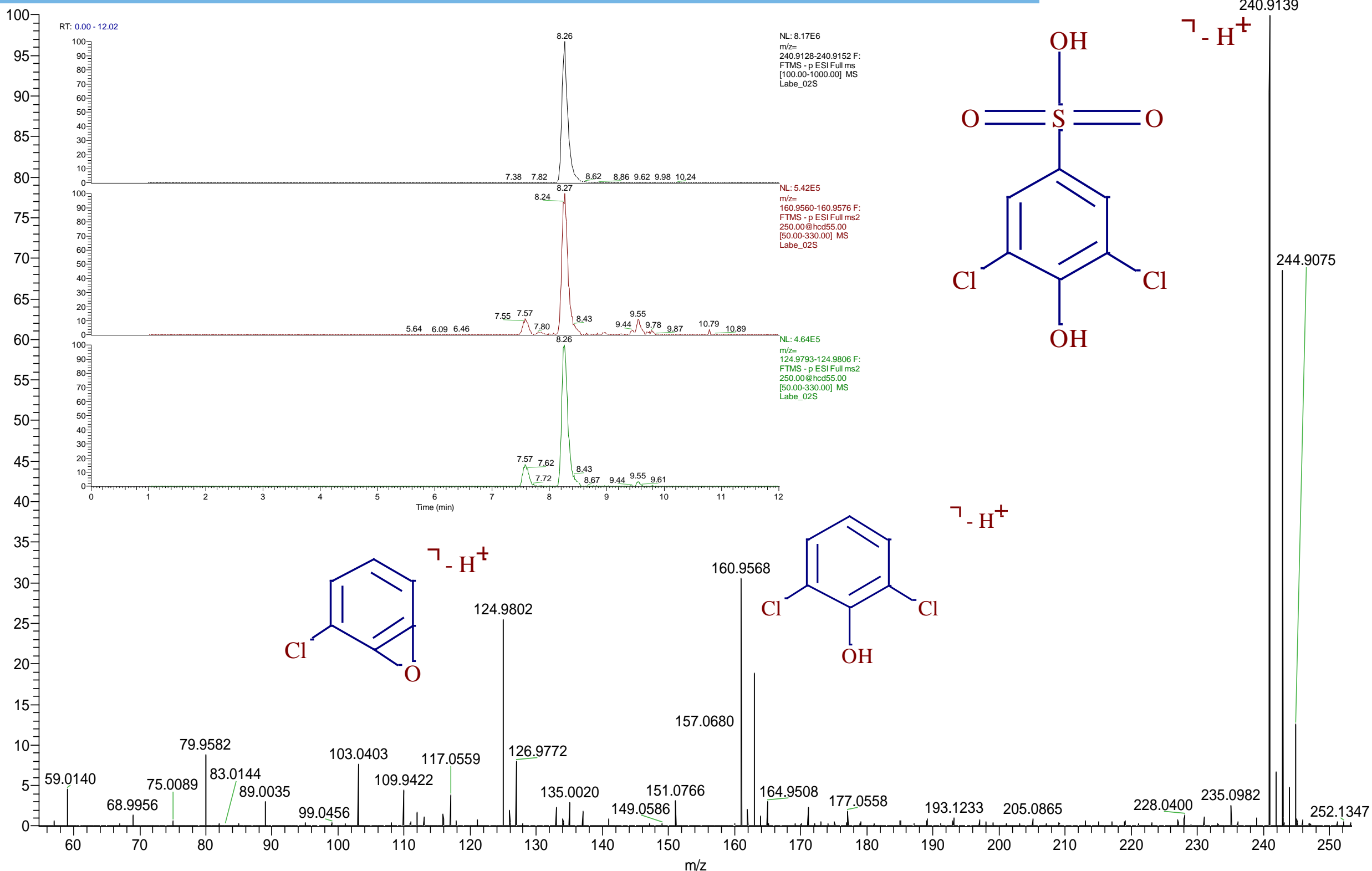


Example 2 CHMI annual surface water quality monitoring



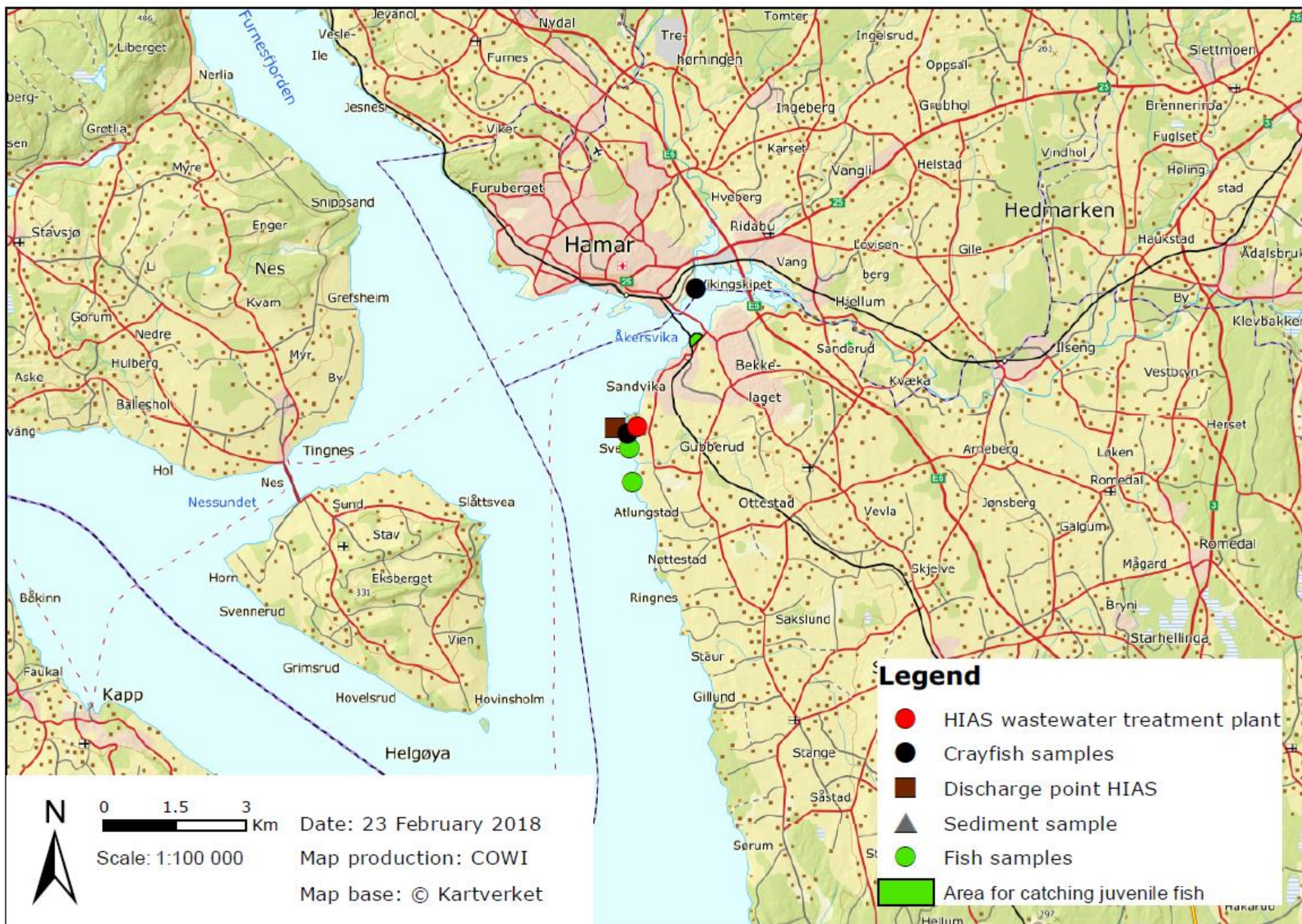


3,5 dichloro – 4 hydroxybenzensulphonic acid





Example 3 screening for new pollutants in lake Mjøsa

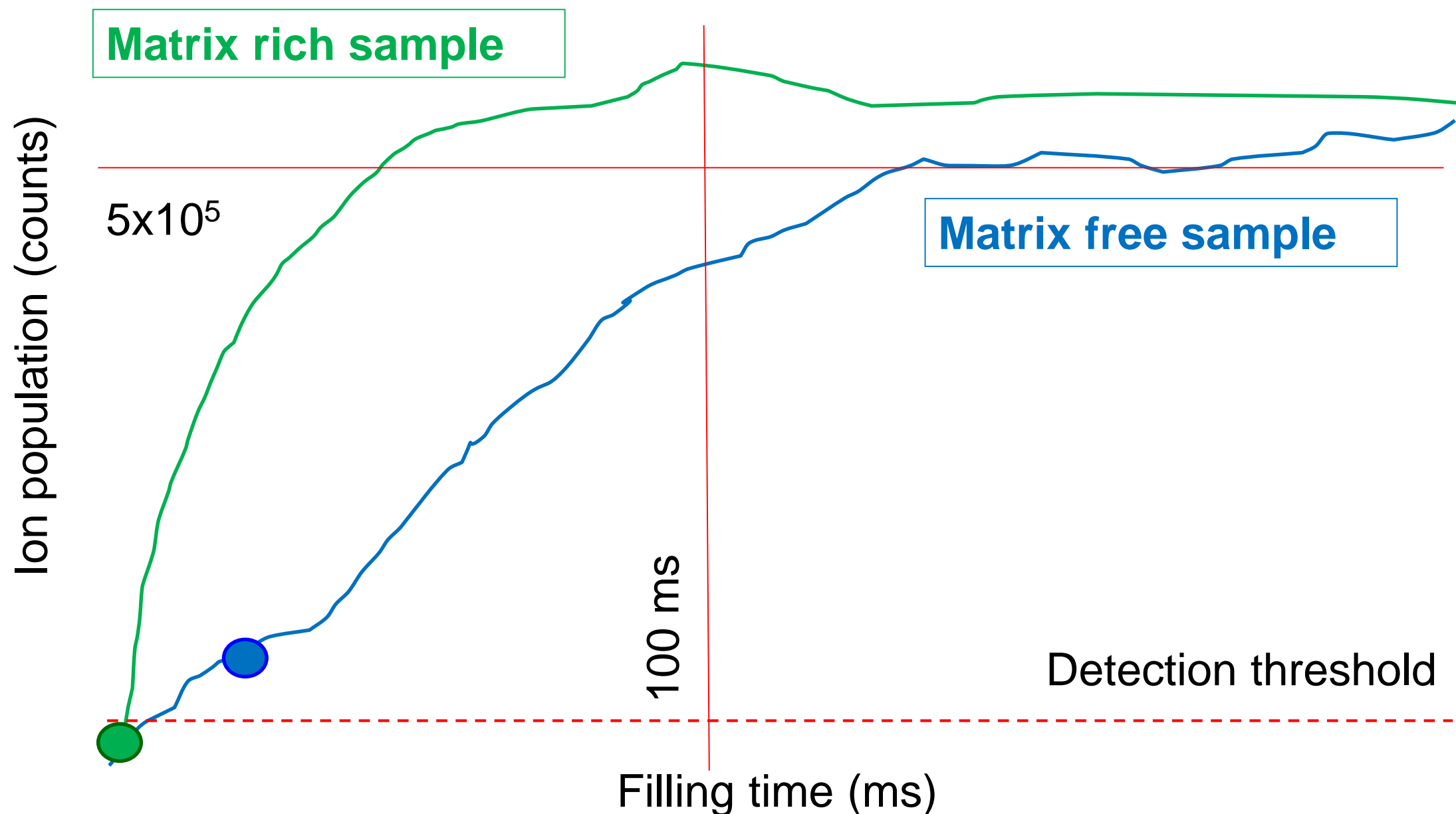




Ions handling and analysis in orbital trap

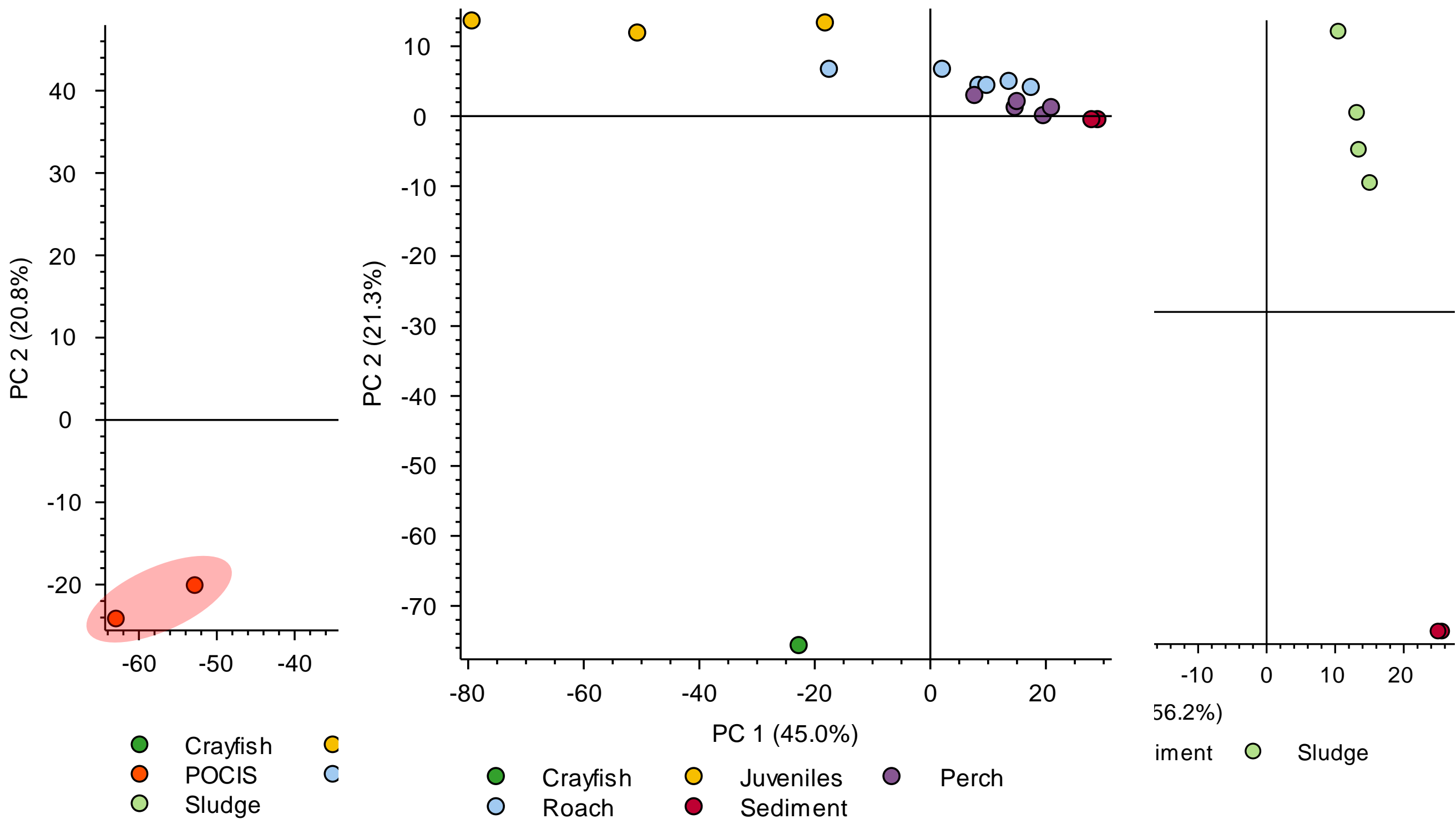
AGS target vs. filling time

Ion population abundance in
Ctrap vs. chromatography





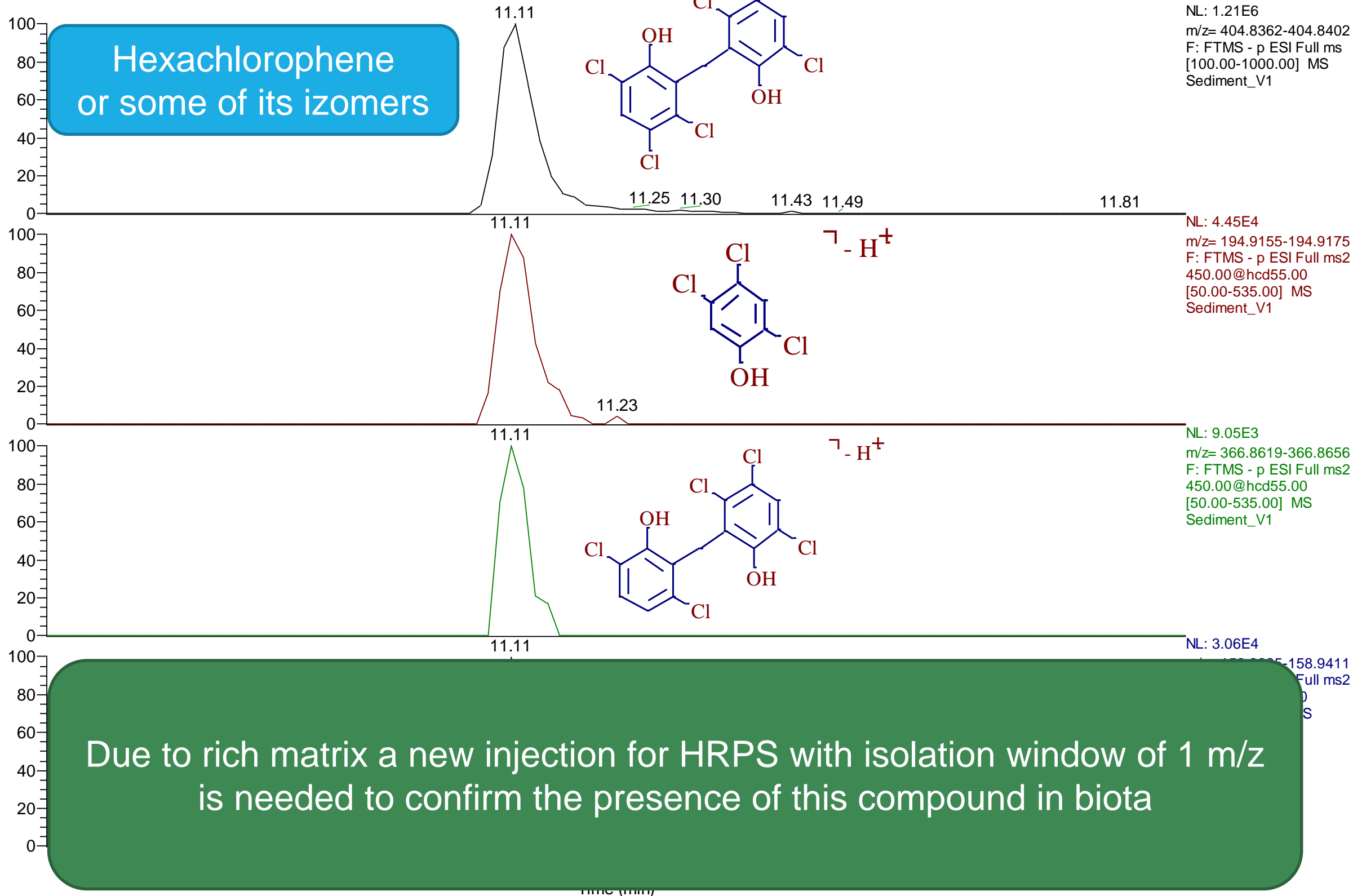
Example 3 screening for new pollutants in lake Mjøsa





Example 3 screening for new pollutants in lake Mjøsa

RT: 10.57 - 11.89





- We can use HRMS signals for descriptive or differential statistical analysis
- Filtration of the data is necessary

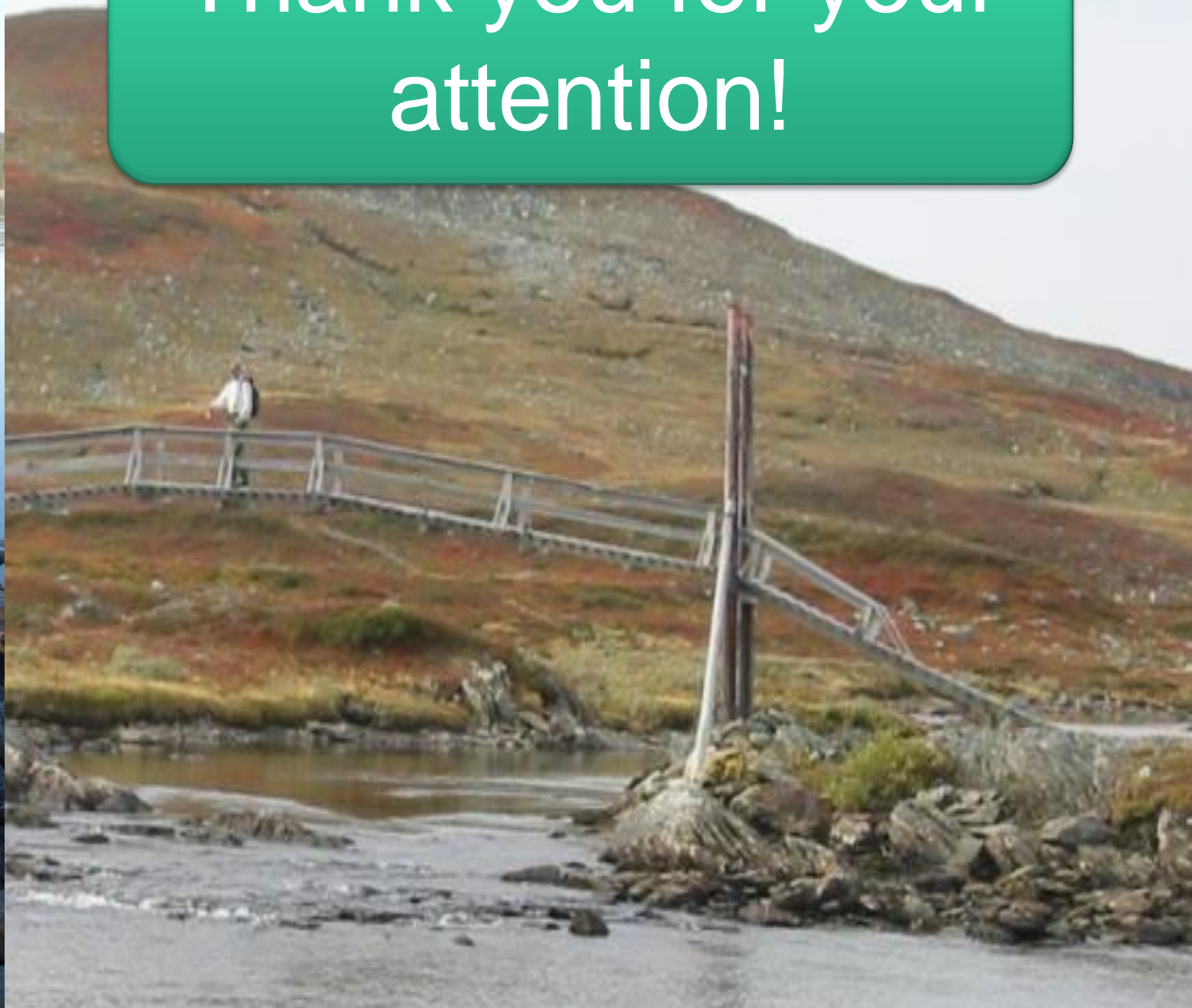
- Definition of the hypothesis prior sampling design is beneficial
- Definition of tested variables is basic assumption of valuable results

- The software has many setup variables – it is important to know how to use them and identify limitations
- All unknown findings must be carefully crosschecked

- Comparing the same matrix – especially matrix free passive samplers – is relatively robust
- Investigation among different matrices remain challenging



Thank you for your attention!



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