Actively searching for pollutants? Screening!

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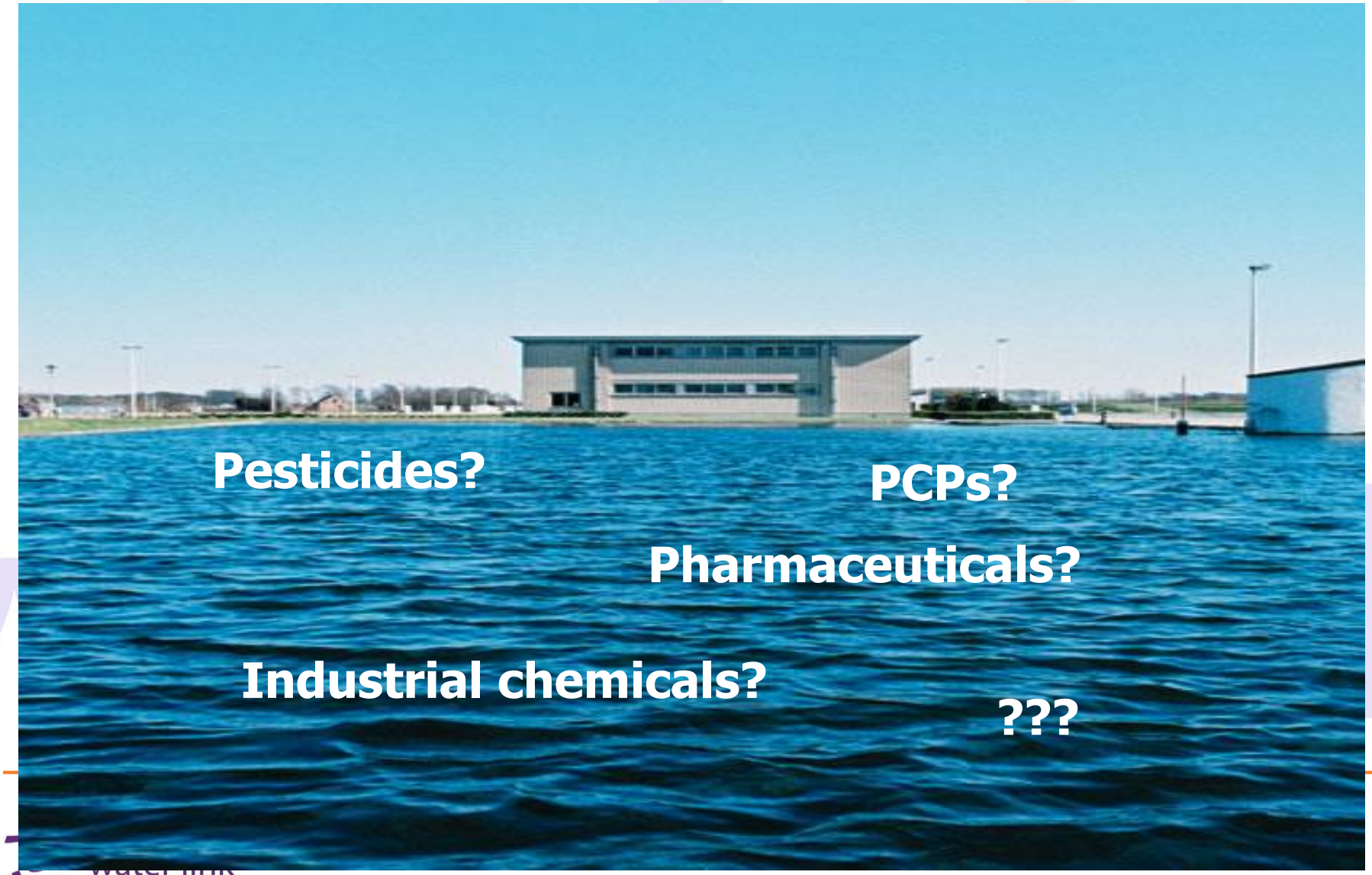
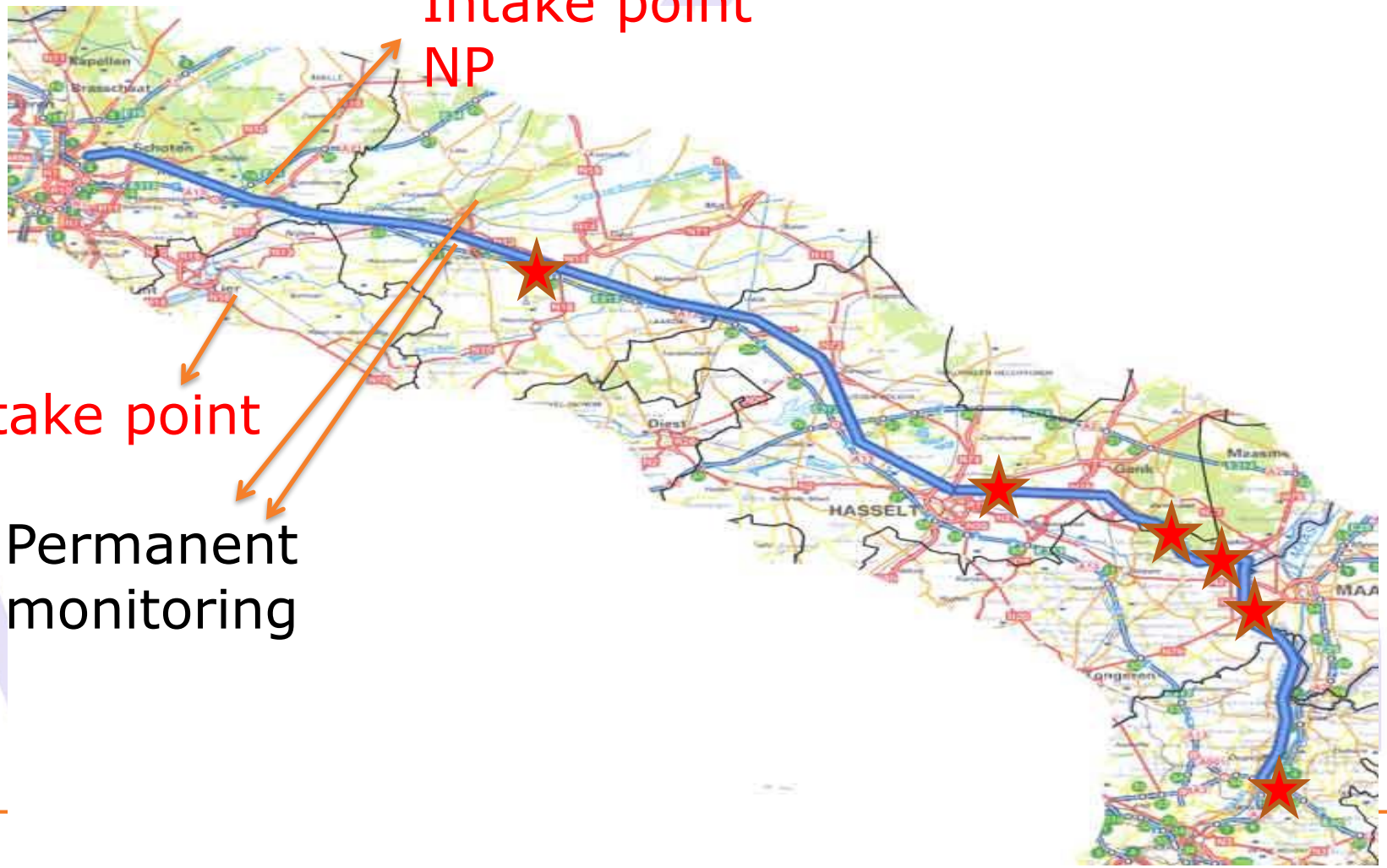
Why screening?



Albert Channel: source of our drinking water



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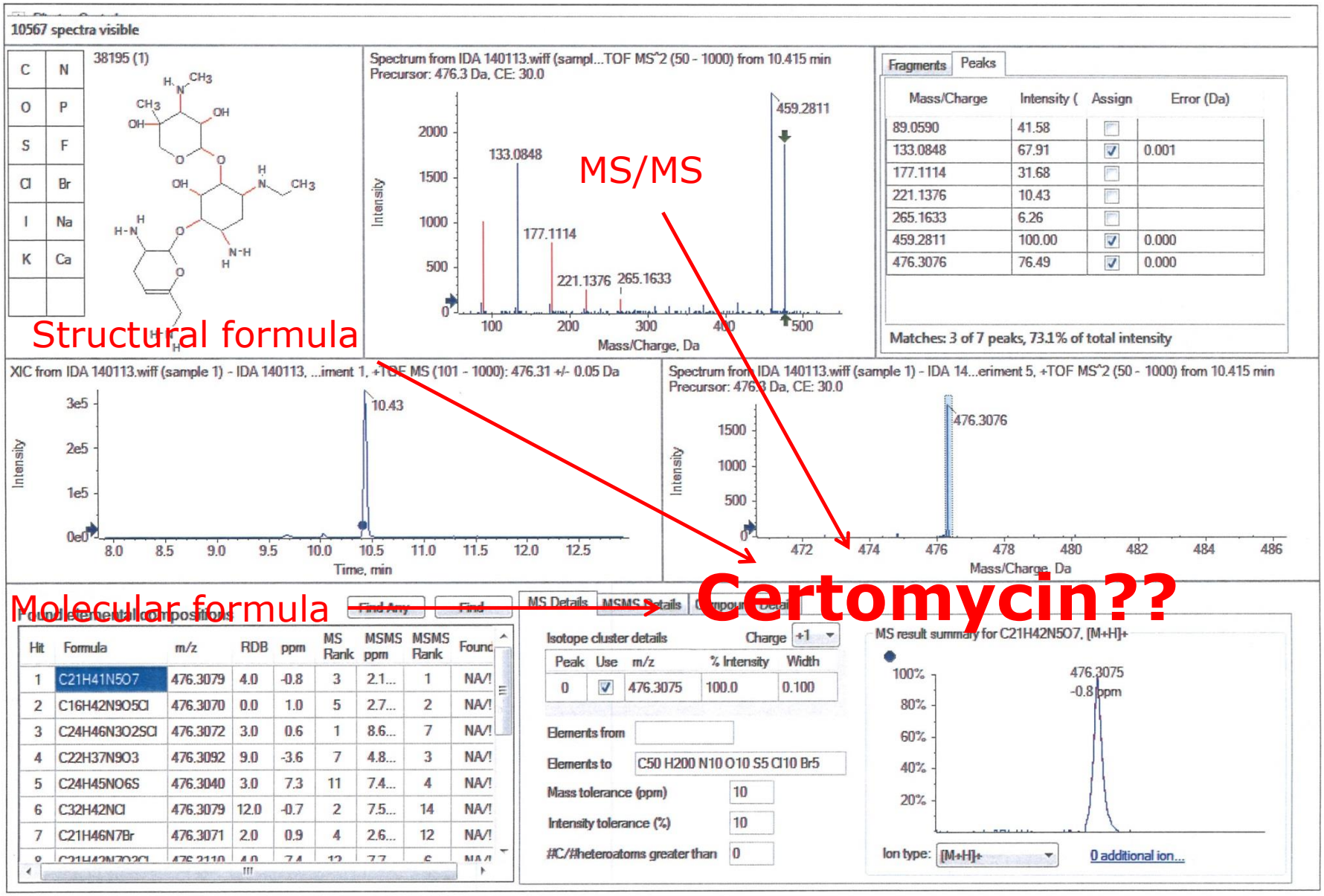
Screening surface water

Metformin	Antidiabeticum	Oxilofrine	Amphetamine analogue
Sulpiride	Antipsychotic drug	Sotalol	Beta blocker
Tramadol	Opioid analgesic	280,21/7,5	
Butetamate	Bronchodilator	Carbamazepine	Antiepelepticum
Flecainide	Antiarrhythmicum	3,4-dimethoxyphenethylamine	Neurotransmitter
192,16/3,5		Eprosartan	Angiotensin receptor blocker
Thymopentin	Immunos...lant	476,31/10,5	
Celiprolol	Beta block...	Viquidil	Antithrombotic drug
Venlafaxine	Antidepressant	Amylocaine	Local anesthetic
Ciclacillin	Antibiotic	Oxibendazole	Veterinary drug
Telmisartan	Angiotensin receptor blocker	Zearalenone	Mycotoxine
Benzoylecgonine	Metabolite of cocaine	Carbendazim	Herbicide
Etilefrine	Antihypotensive cardiac stimulant	Flufenacet	Herbicide
Amisulpride	Antipsychotic	Pethidine	Opioid analgesic
236,19/5,0		Quinidine	Antiarrhythmicum
Cyclopentamine	Vasoconstrictor	Metoprolol	Beta blocker
Thiabendazole	Fungicide	Quinine	Antipyrethroid drug
Valsartan	Angiotensin receptor blocker	Cetobemidone	Opioid analgesic
Lamotrigine	Anticonsulvant		


10567 spectra visible
38195 (1)
Structural formula
Spectrum from IDA 140113.wiff (sampl...TOF MS^2 (50 - 1000) from 10.415 min
Precursor: 476.3 Da, CE: 30.0
459.2811
133.0848
177.1114
221.1376
265.1633
Intensity
Mass/Charge, Da
MS/MS
Fragments
Peaks
Mass/Charge
Intensity (
Assign
Error (Da)
89.0590 41.58
133.0848 67.91 0.001
177.1114 31.68
221.1376 10.43
265.1633 6.26
459.2811 100.00 0.000
476.3076 76.49 0.000
Matches: 3 of 7 peaks, 73.1% of total intensity
XIC from IDA 140113.wiff (sample 1) - IDA 140113, ...iment 1, +TOF MS (101 - 1000): 476.31 +/- 0.05 Da
10.43
Time, min
Spectrum from IDA 140113.wiff (sample 1) - IDA 14...eriment 5, +TOF MS^2 (50 - 1000) from 10.415 min
Precursor: 476.3 Da, CE: 30.0
476.3076
Molecular formula
Certomycin??
Find Any
Find
MS Details
MSMS Details
Hit
Formula
m/z
RDB
ppm
MS Rank
MSMS ppm
MSMS Rank
1 C21H41N5O7 476.3079 4.0 -0.8 3 2.1... 1 NA/!
2 C16H42N9O5Cl 476.3070 0.0 1.0 5 2.7... 2 NA/!
3 C24H46N3O2SCl 476.3072 3.0 0.6 1 8.6... 7 NA/!
4 C22H37N9O3 476.3092 9.0 -3.6 7 4.8... 3 NA/!
5 C24H45NO6S 476.3040 3.0 7.3 11 7.4... 4 NA/!
6 C32H42NCl 476.3079 12.0 -0.7 2 7.5... 14 NA/!
7 C21H46N7Br 476.3071 2.0 0.9 4 2.6... 12 NA/!
Isotope cluster details
Charge +1
Peak Use m/z % Intensity Width
0 476.3075 100.0 0.100
Elements from
Elements to C50 H200 N10 O10 S5 Cl10 Br5
Mass tolerance (ppm) 10
Intensity tolerance (%) 10
#C/#heteroatoms greater than 0
MS result summary for C21H42N5O7, [M+H]+
476.3075
-0.8 ppm
Ion type: [M+H]+
0 additional ion...

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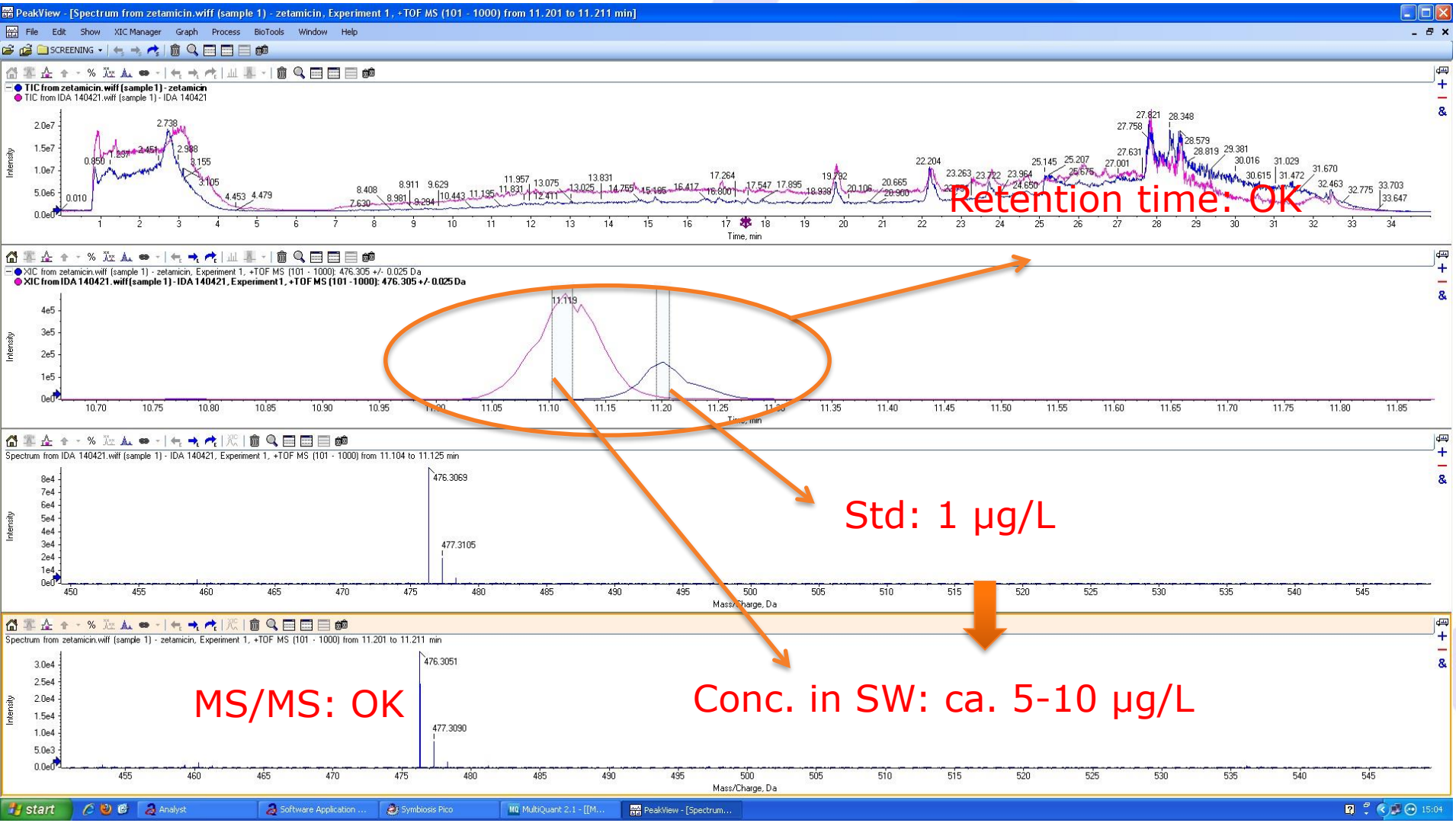
BUT:

- Compound is not commercially available in Belgium
- Certomycine is not medically applied in Belgium
- Hence: wrong conclusion…?
- We found the product in Italy and injected it on our instrument…


PeakView - [Spectrum from zetamicin.wiff (sample 1) - zetamicin, Experiment 1, +TOF MS (101 - 1000) from 11.201 to 11.211 min]
Retention time: OK
Std: 1 µg/L
Conc. in SW: ca. 5-10 µg/L
MS/MS: OK
476.3051
477.3090
Mass/Charge, Da

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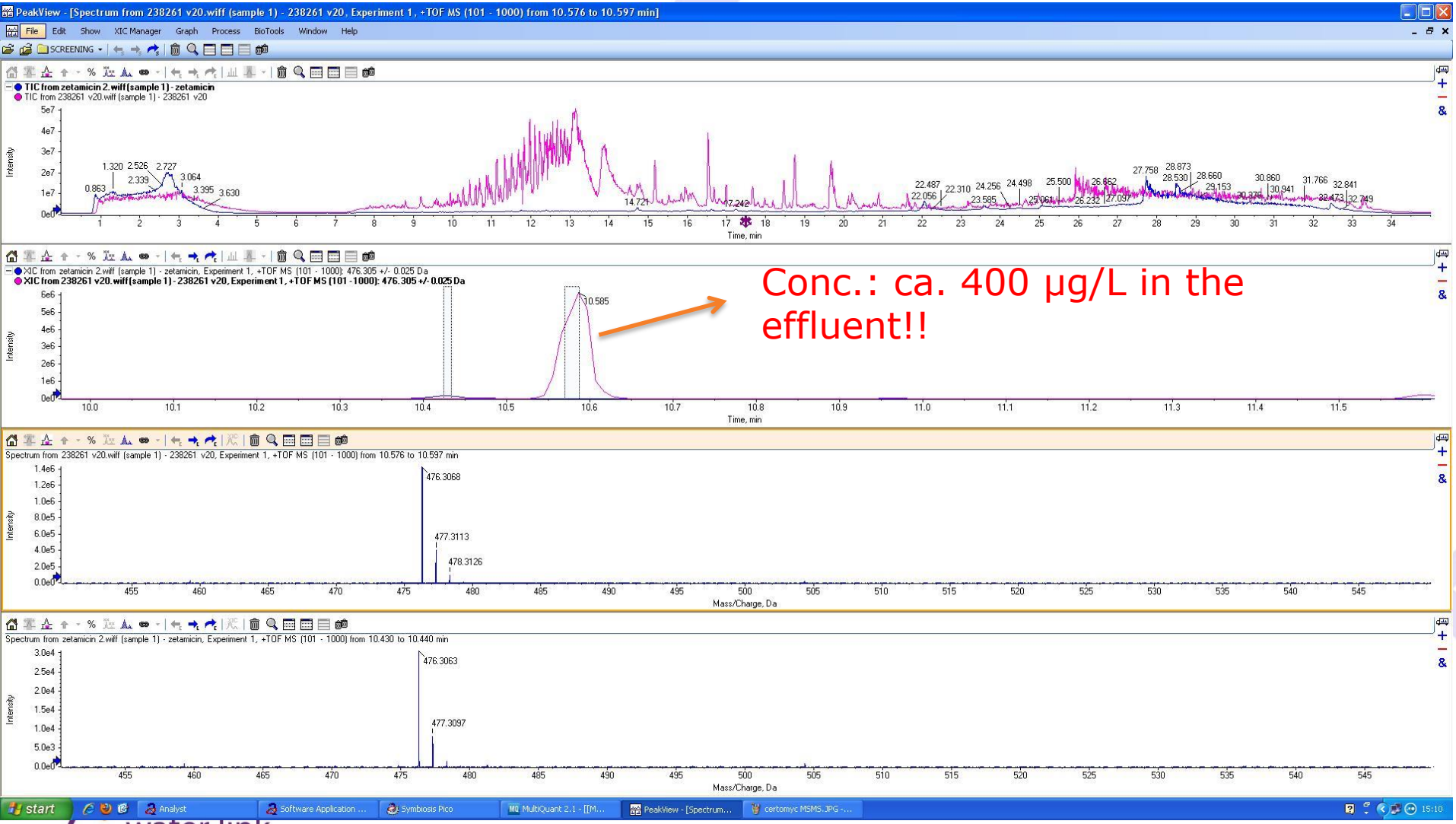
Veal butchery effluent?



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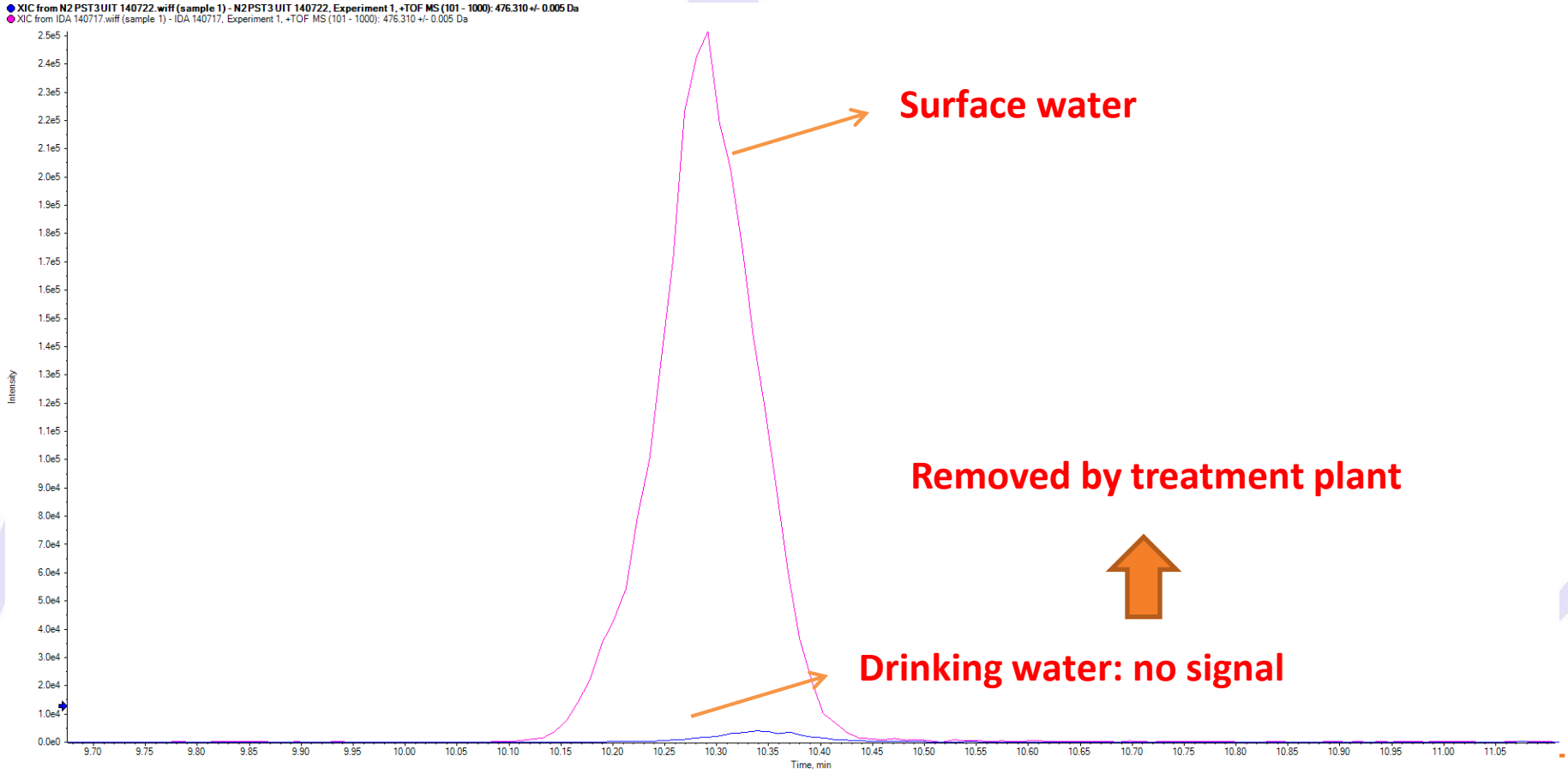
Status drinking water??



Besluit

- Screening is very important to actively searching for pollutants in surface and drinking water.
- Screening can help in finding sources of pollution.

- More information: www.water-link-laboratory.com