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Predicting formation of disinfection by-products under Climate Change uncertainties

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Water Harmony

International Symposium "Water Resources Management: New Perspectives and Innovative Practices„
Novi Sad, 23-24 September 2021

Water Harmony research group

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Environmental & Industrial Process Analytics

Smart Water Quality Monitoring
- Soft sensors for nutrients and contaminants of emerging concern
- Sensor fusion

Process Surveillance and Control
- Data Mining and Big Data Analytics
- Machine learning and ANN
- Digital water security
- Real-time Predictive Analytics
- Image analysis in process surveillance

Advanced Water & Wastewater Treatment

Coagulation & Flocculation
- State-of-the-art coagulation control
- Fusion of coagulants
- Nature-derived reagents
- Increasing fertiliser value of coagulated sludge

Membrane Separation
- Ceramic Membrane Biological Reactor
- Nanofiltration for surface water treatment
- Reverse Osmosis for groundwater treatment

Electrochemical Methods
- Electrocoagulation
- Electrooxidation of Contaminants of Emerging Concern

Why?

Climate Change → Natural Organic Matter (NOM) → Oxidative disinfection → Disinfection by-products (DBPs)

Disinfection by-products (DBPs)

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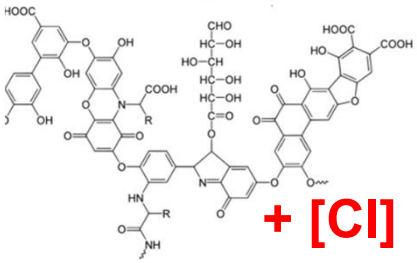

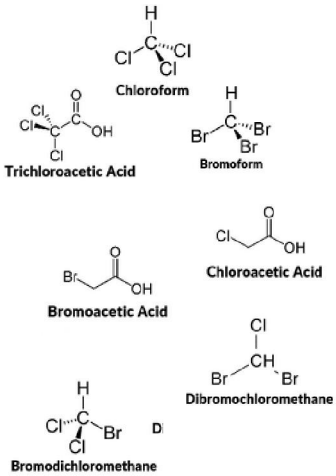

Lee, Kim, et al., 2013

Luben, Olshan, et al., 2013

Kogevinas, Villanueva, et al., 2010

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NOM concentration is increasing

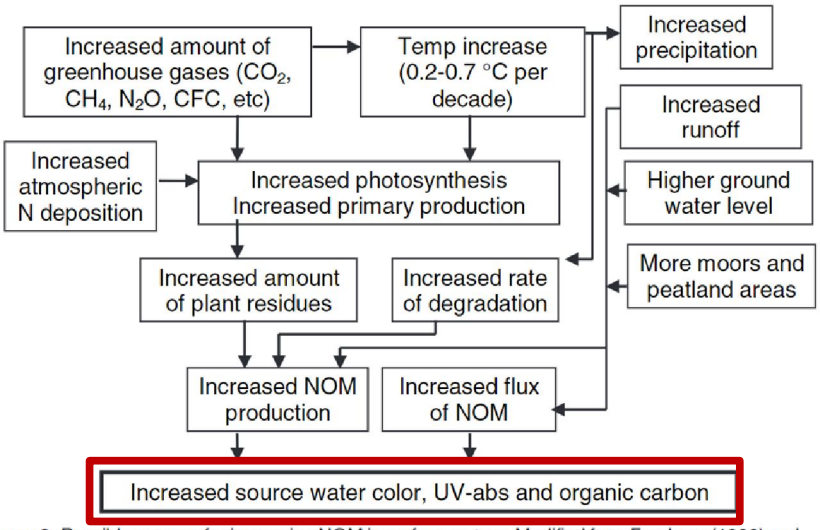

Figure 2 Possible reasons for increasing NOM in surface waters. Modified from Forsberg (1992) and Liltved (2002)

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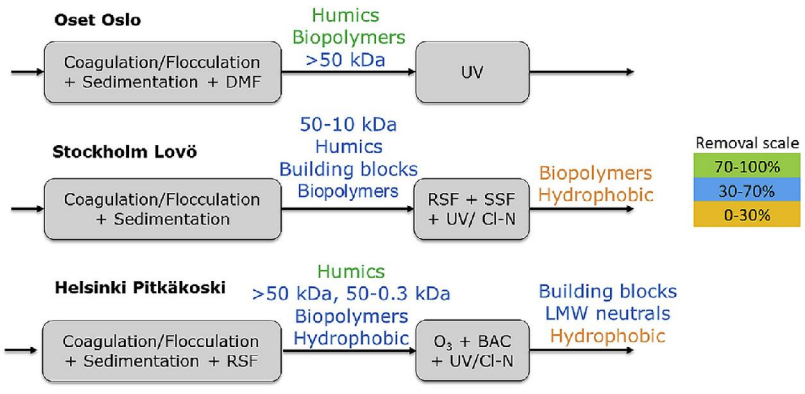
Climate Change and NOM in surface water



Remaining NOM: high MW fraction >50kDa (55-80%), consisting of humics (33-62%), building blocks (14-30%) and LMW neutrals (7-17%)

P.Krzeminski[a] C.Vogelsang[a] T.Meyn[b] S.J.Köhler[c] H.Poutanen[d] H.A.de Wit[a] W.Uhl[ab]

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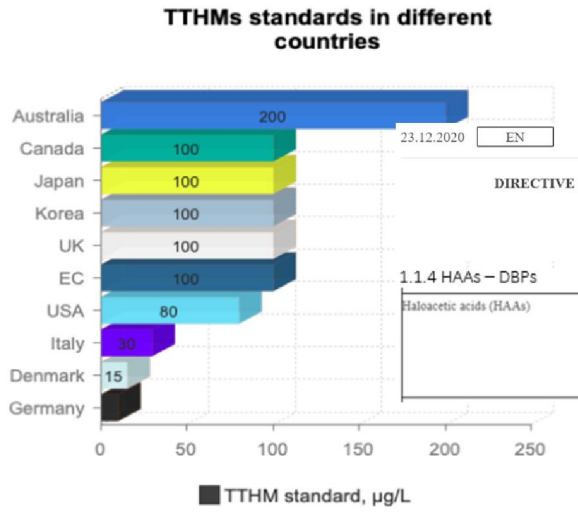
Legal requirements



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of 16 December 2020

on the quality of water intended for human consumption

1.1.4 HAAs – DBPs

Haloacetic acids (HAAs)	60	µg/l	This parameter shall be measured only when disinfection methods that can generate HAAs are used for the disinfection of water intended for human consumption. It is the sum of the following five representative substances: monochloro-, dichloro-, and trichloro-acetic acid, and mono- and dibromo-acetic acid.

Bond, Goslan, et al., 2012

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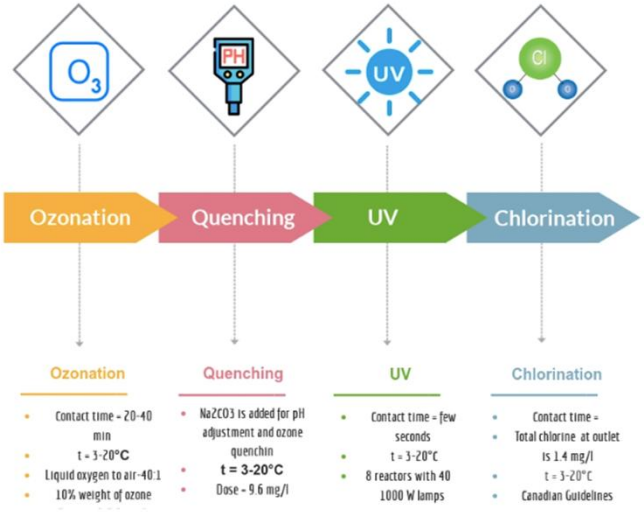
Study case



Can we predict DBPs based on raw water and process parameters?

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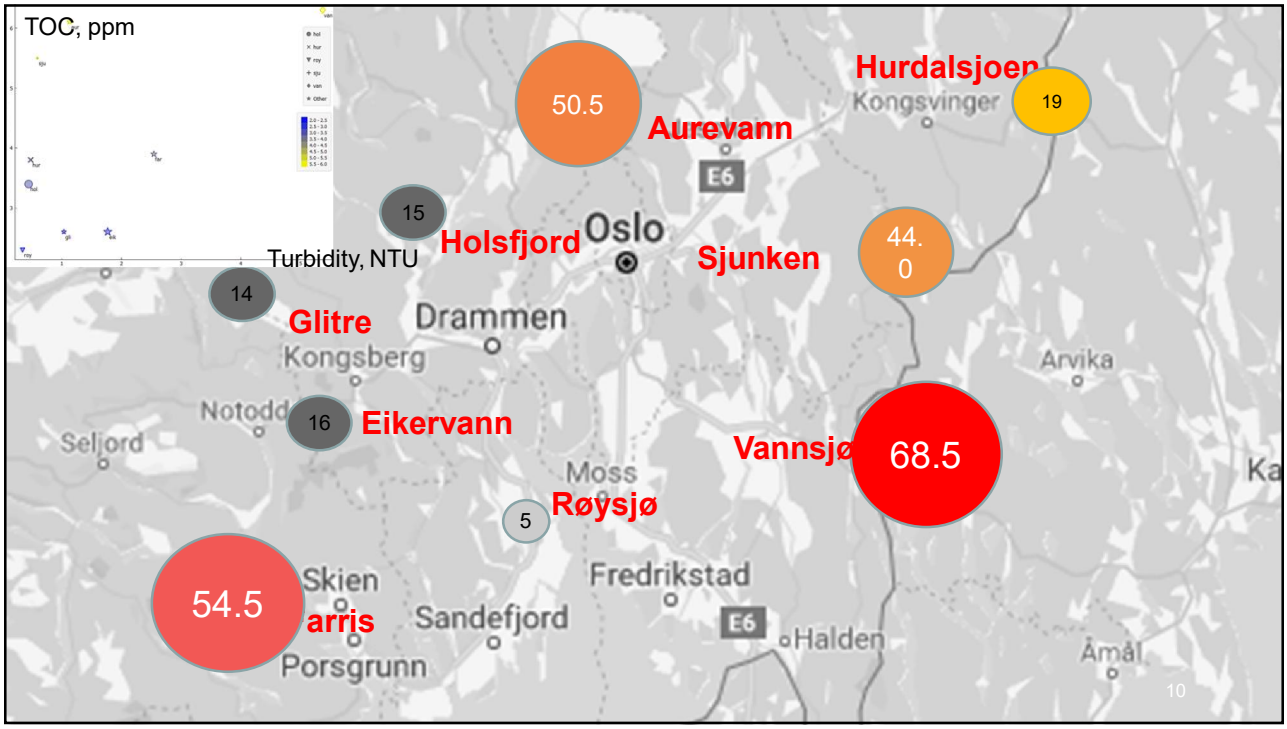
Lillehammer
Gjøvik
Hamar
Elverum
Hurdalsjøen
Aurevann
Holsfjord
Sjunken
Glitre
Oslo
Drammen
Kongsberg
Eikervann
Røysjø
Vannsjø
Moss
Fredrikstad
Skien
Sandefjord
Farris
Halden
Arvika
Karlstad
Malung
Mora
Rjukan
Arendal
Grimstad
Kristiansand
Trollhättan kommune


TOC, ppm
Turbidity, NTU
50.5
Aurevann
Hurdalsjoen
Kongsvinger
19
E6
15
Holsfjord
Oslo
Sjunken
44.0
14
Glitre
Drammen
Kongsberg
Arvika
Notodden
16
Eikervann
Seljord
Vannsjø
68.5
Moss
Røysjø
5
54.5
Skien
arris
Sandefjord
Fredrikstad
E6
Halden
Porsgrunn
Åmål
10

Dataset

Water

Source *(category)*:
- aur
- eik
- far
- gli
- hol
- hur
- roy
- sju
- van

Raw

Quality *(features)*:
- pH
- Turb
- Color
- TOD
- TOC
- SUVA
- UV254

THFMP tests *(features)*:
- $THMFP_t$
- THM_t
- FRC_t

Treated

Quality *(features)*:
- UV254
- THM

UV-VIS spectra

Treatment parameters (factors)
- O3
- Time
- Cl

Study scheme

Sampling
- aur
- eik
- far
- gli
- hol
- hur
- roy
- sju
- van

1

Analysis
- pH
- Turb
- Color
- TOD
- TOC
- SUVA
- UV254
- *UV-VIS spectra*

2

THMFP tests

Results:
- $THMFP_t$
- THM_t
- FRC_t

3

Disinfection tests

+ O_3	+ Time	+ Cl
1,5 3	15 45	2

Results:
- THM
- UV254
- *UV-VIS spectra*

Research questions:

1.1 Which minimal analysis data can be used to identify the source of water for unknown samples accurately?

1.2 Can difficult-to-measure ***off-line*** parameters (TOD, TOC, SUVA) be estimated through easy-to-measure ***at-line*** parameters (Color, UV254) and ***in-line*** parameters (pH, Turb, UV-VIS spectrum)

2.1 Which minimal analysis data can be used to predict results of THMFP tests:
- ***in-line*** parameters (pH, Turb, UV-VIS spectrum)
- ***at-line*** parameters (Color, UV254)
- ***off-line*** parameters (TOD, TOC, SUVA)

3.1 Is there a model to maintain THM ≤ 50 by varying O_3 and Time for water with specific parameters?

3.2 Are there characteristic changes in UV-VIS spectra of raw and treated water that can be used to predict THM in treated water?

Analysed parameters

Correlation coefficients									
Parameters	**THM**	**SUVA**	**Color**	**TU**	**COND.**	**pH**	**TOD**	**TOC**	**UV $_{254}$**
THM	1								
SUVA	0.74	1							
Color	0.85	**0.92**	1						
TU	0.64	0.83	0.79	1					
COND.	0.59	0.74	0.81	0.85	1				
pH	0.07	0.12	-0.07	0.20	-0.20	1			
TOD	**0.93**	0.85	**0.91**	0.76	0.80	-0.08	1		
TOC	**0.92**	0.74	0.88	0.57	0.69	-0.23	**0.95**	1	
UV $_{254}$	**0.91**	**0.90**	**0.96**	0.81	0.83	-0.08	**0.98**	**0.94**	1

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Spectra – Big Data

A	B	C	D	E	F	G	H	
Sample ID	**Source**	**Ozone**	**Time**	**Chlorine**	**pH-raw**	**Turb-raw**	**Color-raw**	**Conc**
aur-0-0-0	aur	0	0	0	6,561	1,13	50,5	4
aur-0-0-2	aur	0	0	2	6,561	1,13	50,5	4
aur-0-0-6	aur	0	0	6	6,561	1,13	50,5	4
aur-15-15-2	aur	1,5	15	2	6,561	1,13	50,5	4
aur-15-45-2	aur	1,5	45	2	6,561	1,13	50,5	4
aur-3-15-2	aur	3	15	2	6,561	1,13	50,5	4

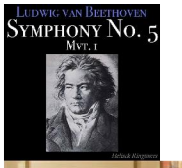
16 variables

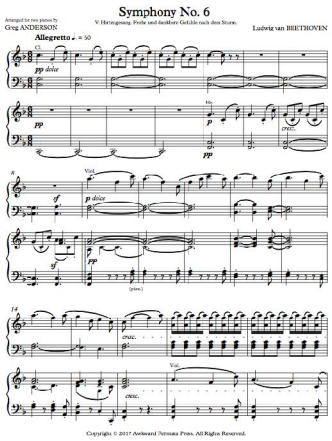
1300 variables

Sample ID	840	839,5	839	838,5	838	837,5
aur-0-0-0	0,00135	0,0013	0,00135	0,00095	0,001	0,00115
aur-15-15-2	0,00075	0,00095	0,0008	0,0008	0,00065	0,00085
aur-15-45-2	0,0025	0,0027	0,0026	0,00255	0,00275	0,00295
aur-3-15-2	0,0017	0,0015	0,0017	0,002	0,0018	0,0018
aur-3-45-2	0,0008	0,0007	0,0009	0,001	0,0008	0,0007

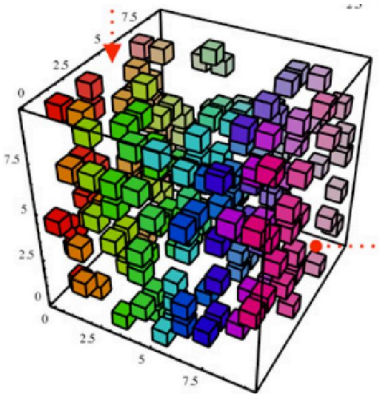
1316 variables

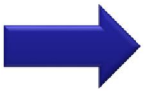
How to extract important information?

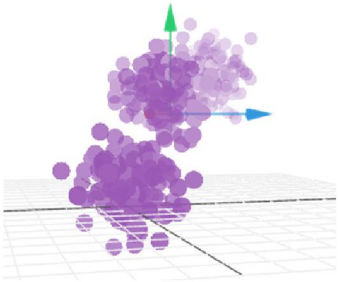




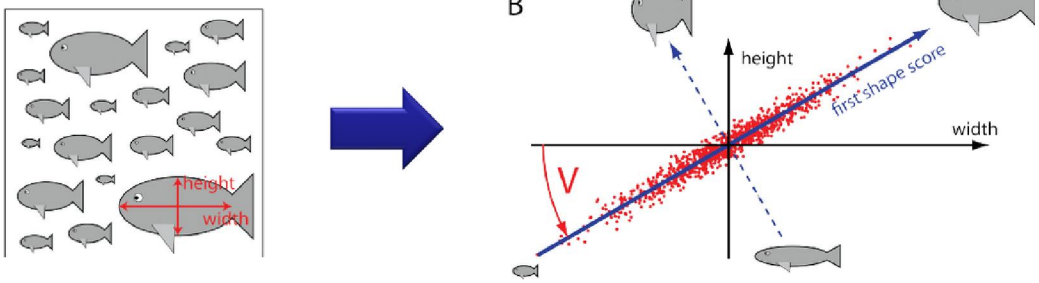
How to extract important information?



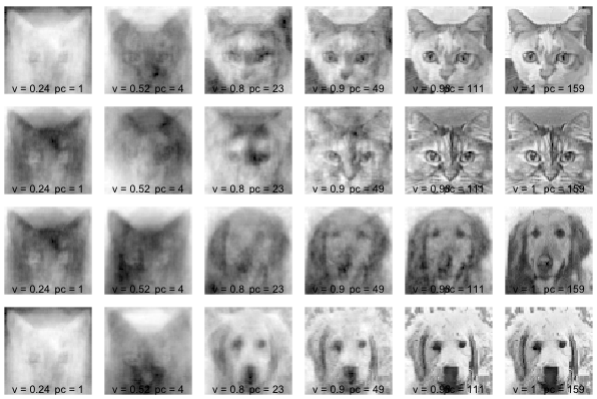




How to extract important information?



How to extract important information?

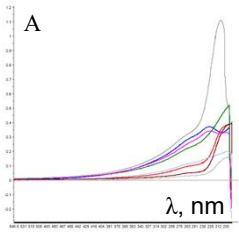


How to extract important information?

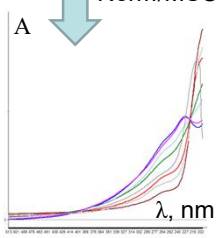
Dimensionality reduction

- Feature Elimination
- **Feature Extraction**
  - We transform the original set of features into another set of features
  - The idea is to pack the most important information into as few derived features as possible
  - **Derived features are a linear combination of the original features**

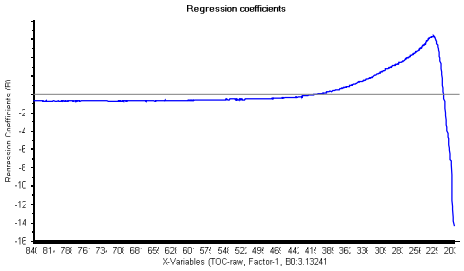
From UV-VIS to TOC

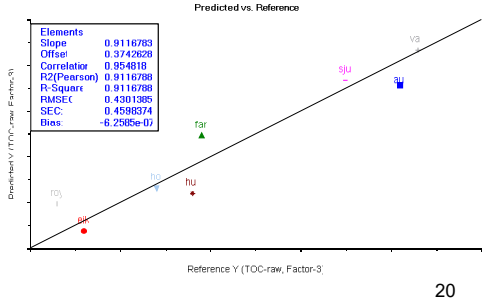


Norm/MSC/SmoothingSG



PLSR





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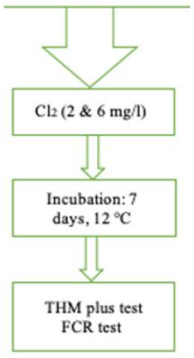
THM Formation Potential (HACH)

- Worst case scenario – 7 days incubation time
- Function of chlorine dose, TOC, temperature, reaction time, and pH
- Can be used for both design & operation of water treatment system
- Helps to get an idea of the THM max possible concentration



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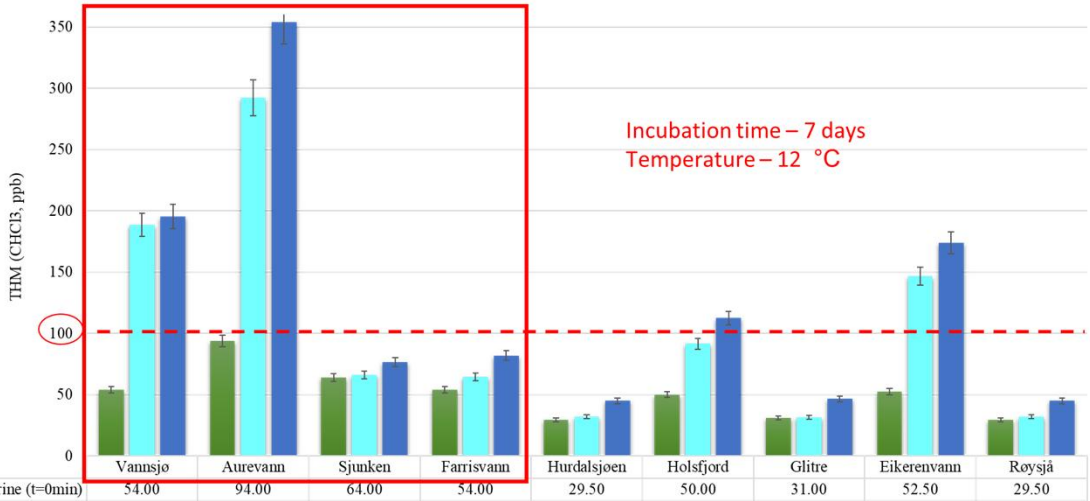
THM Formation Potential (HACH)



	Vannsjø	Aurevann	Sjunken	Farrisvann	Hurdalsjøen	Holsfjord	Glitre	Eikerenvann	Røysjå
2 mg/l Chlorine (t=0min)	54.00	94.00	64.00	54.00	29.50	50.00	31.00	52.50	29.50
2 mg/l Chlorine	188.50	292.50	66.00	64.50	32.00	91.50	31.50	146.50	32.00
6 mg/l Chlorine	195.50	354.00	76.50	82.00	45.00	112.50	46.50	174.00	45.00

* - This table includes average data from duplicate experiments

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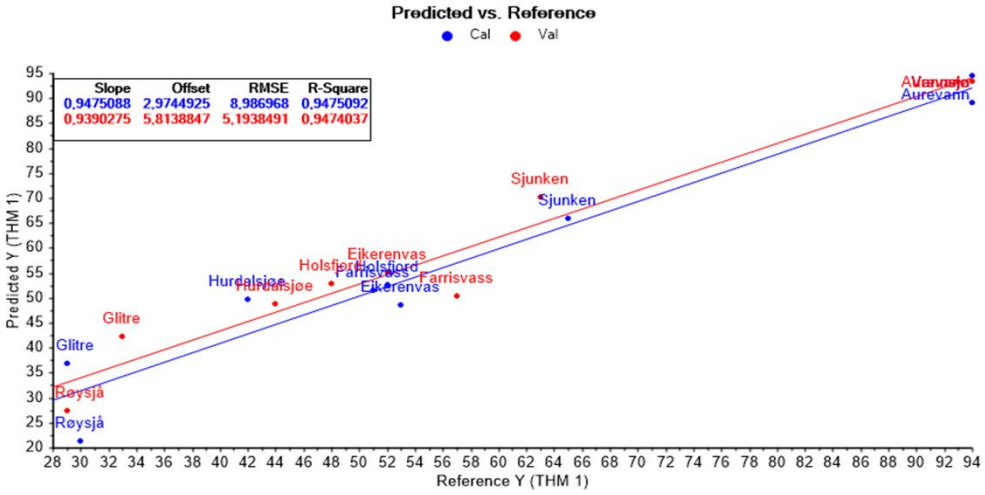
1. Multiple Linear Regression (MLR) for simple water quality parameters



THMFP = -142.66 + 626.24**[UV254]** + 21.90**[pH]** + 4.97**[Turbidity]** - 0.05**[Conductivity]** - 2.02**[Colour]**

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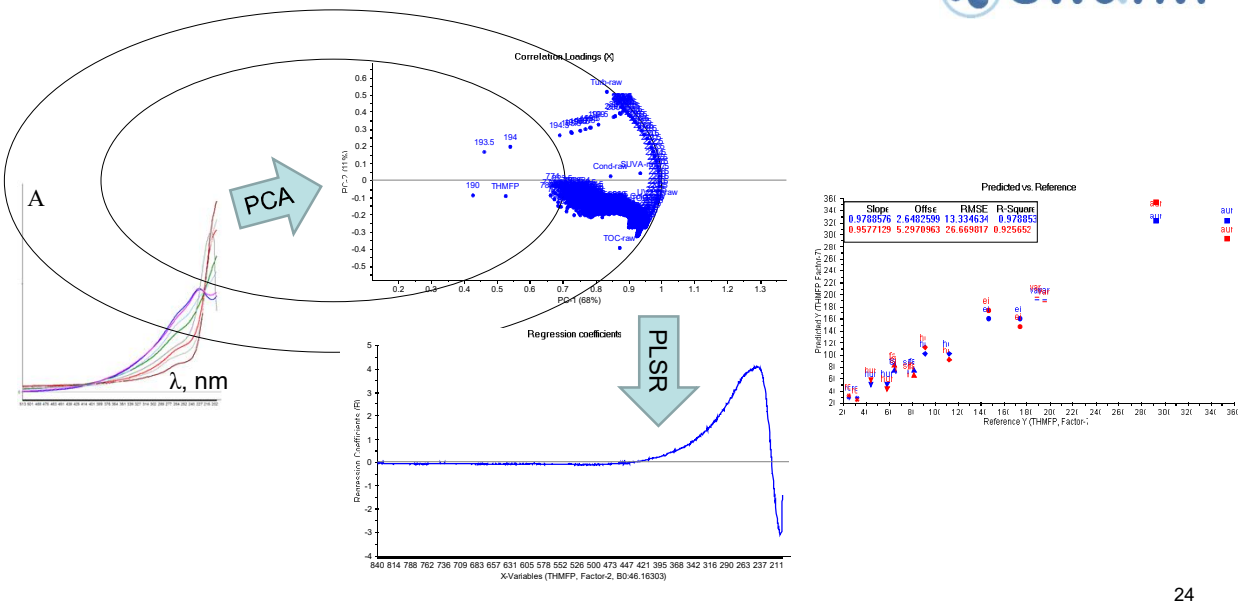
THM Formation Potential



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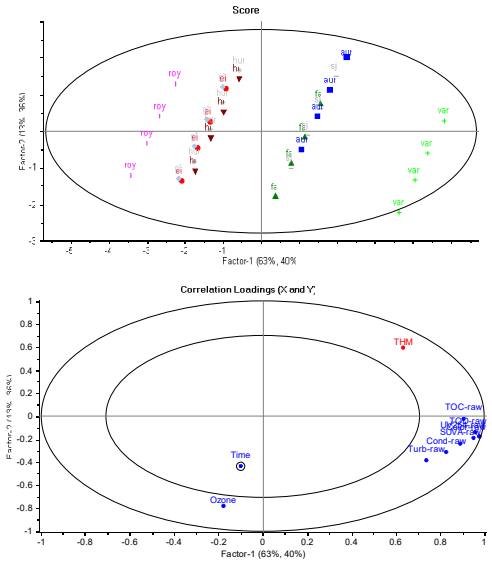
THM concentration in effluent



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Conclusions

- **<u>Climate Change</u>** will continue influencing NOM content in surface water, incl. cold climate zones
- This will **<u>increase risks of exposure to DBPs</u>**, incl. THMs
- **<u>Rapid and online methods of DBPs surveillance</u>** are desired in order to establish analysis routines and improve process control
- **<u>UV-VIS online spectroscopy</u>** together with simply measured parameters can help to estimate THMFP and THM concentration in effluent
- **<u>Alarms over control limits</u>** may trigger lab analysis or control measures

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