

Single Particle ICP-MS and the Quest for Marine Nanoparticles



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#data science #cheminformatics #emerging contaminants
slides: arebruvold.com/research.html



Single Particle ICP-MS and the Quest for Marine Nanoparticles

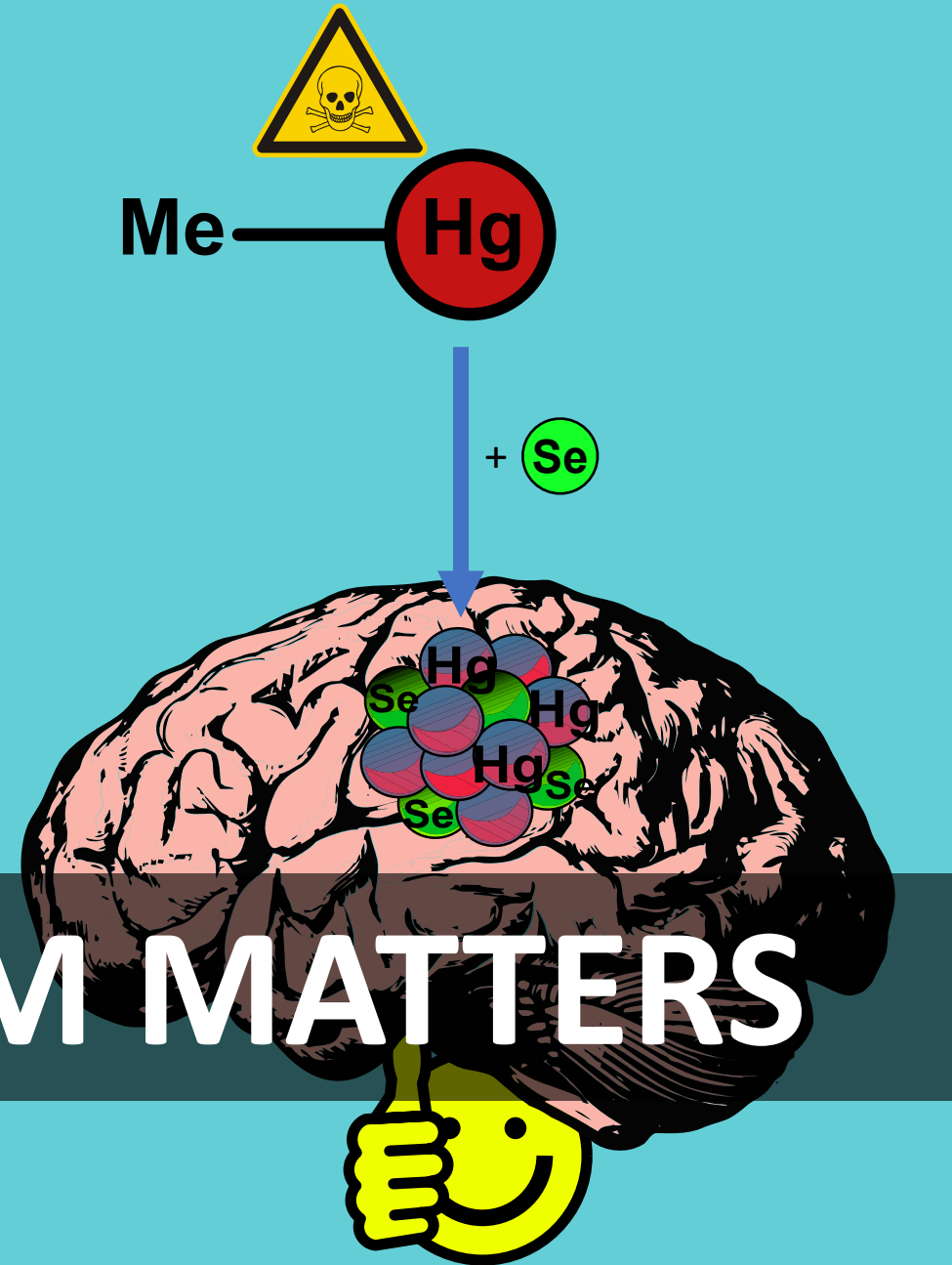


Which would you rather have in your brain?



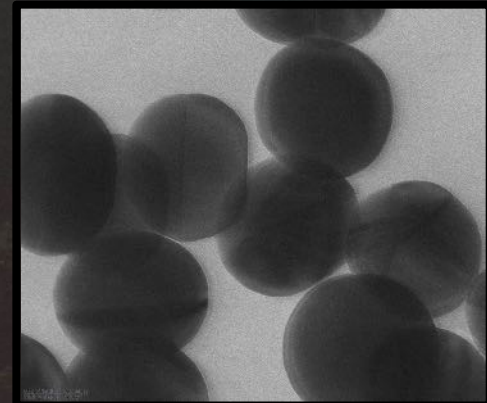
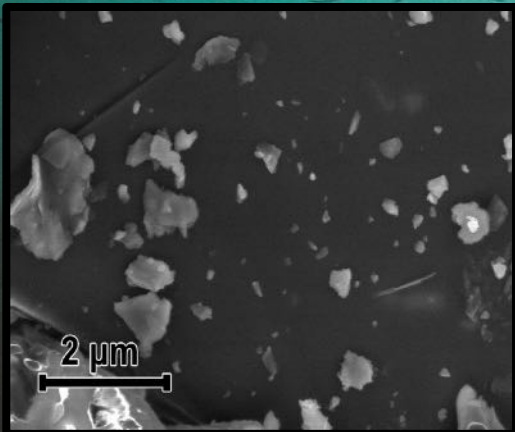
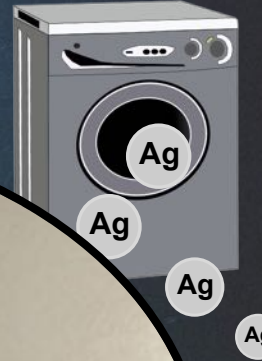
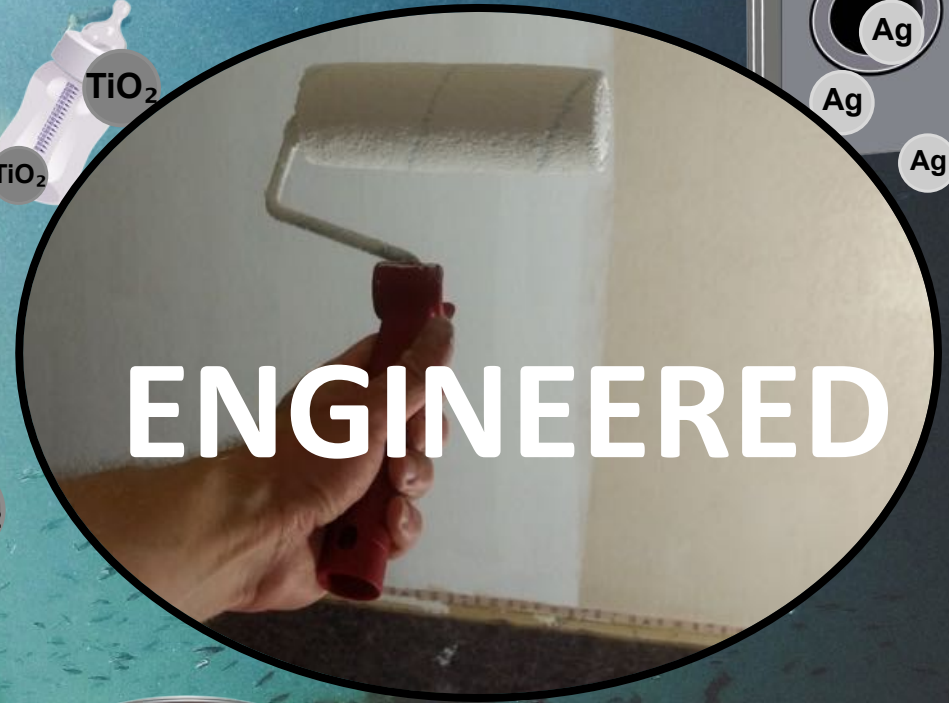
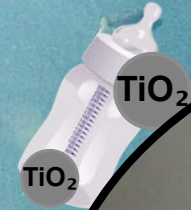


United States Geological Survey CC BY 2, upscaled.



SIZE AND FORM MATTERS

ANTHROPOGENIC NANOPARTICLES



ANTHROPOGENIC NANOPARTICLES



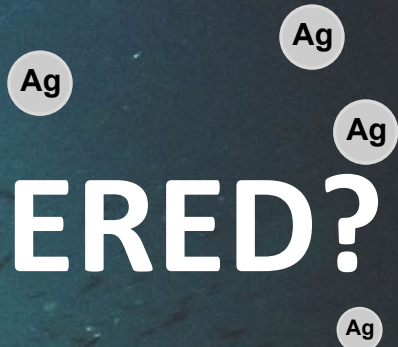
INCIDENTAL?

*Megatons
per year in
NO(?)*

ENGINEERED?

*Qualitative
production data
only.*

vs NATURAL?



ANTHROPOGENIC NANOPARTICLES



INCIDENTAL?

ENGINEERED?

DATA NEEDED

*Megatons
per year in
NO(?)*

*Qualitative
production data
only.*

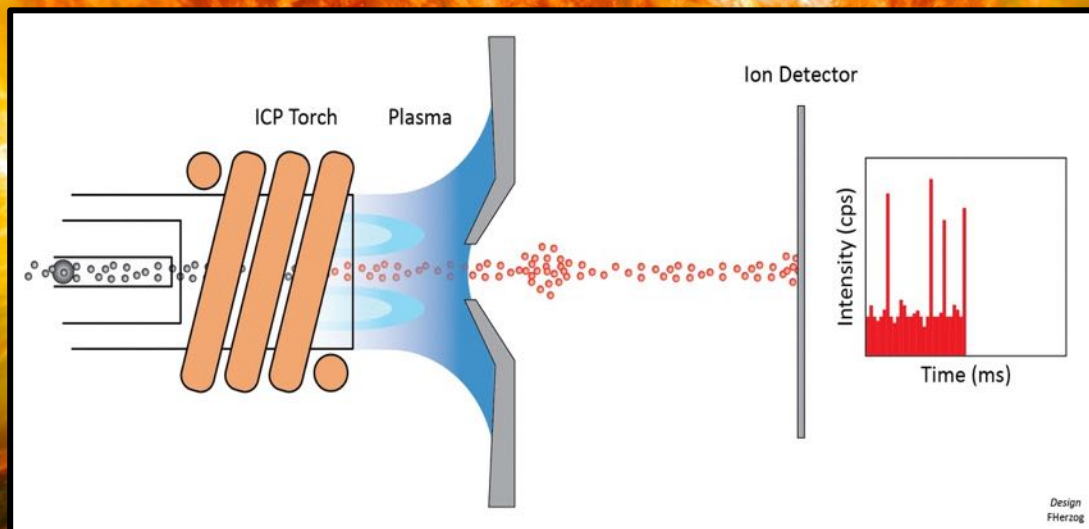
vs NATURAL?



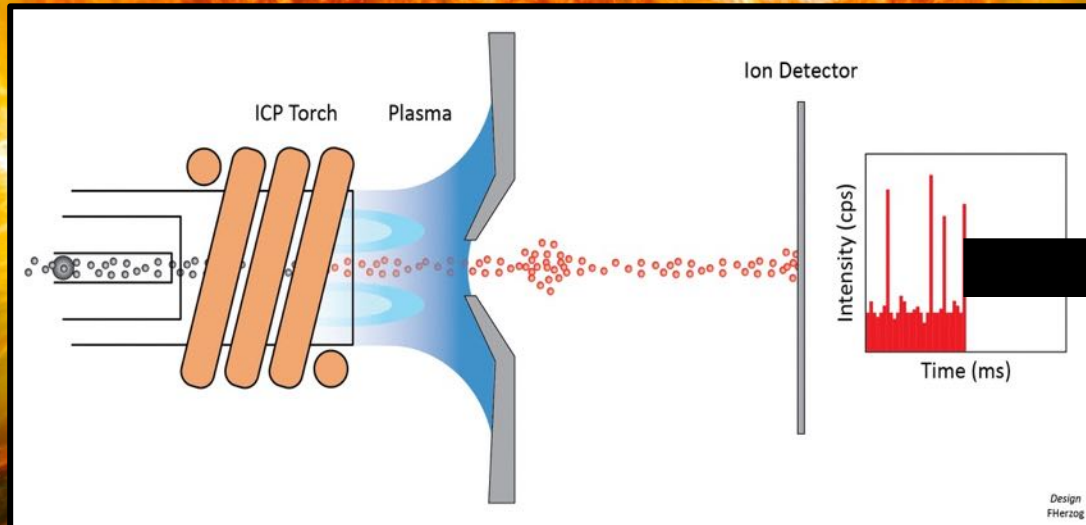
METHODS?



Single Particle ICP-MS



Single Particle ICP-MS

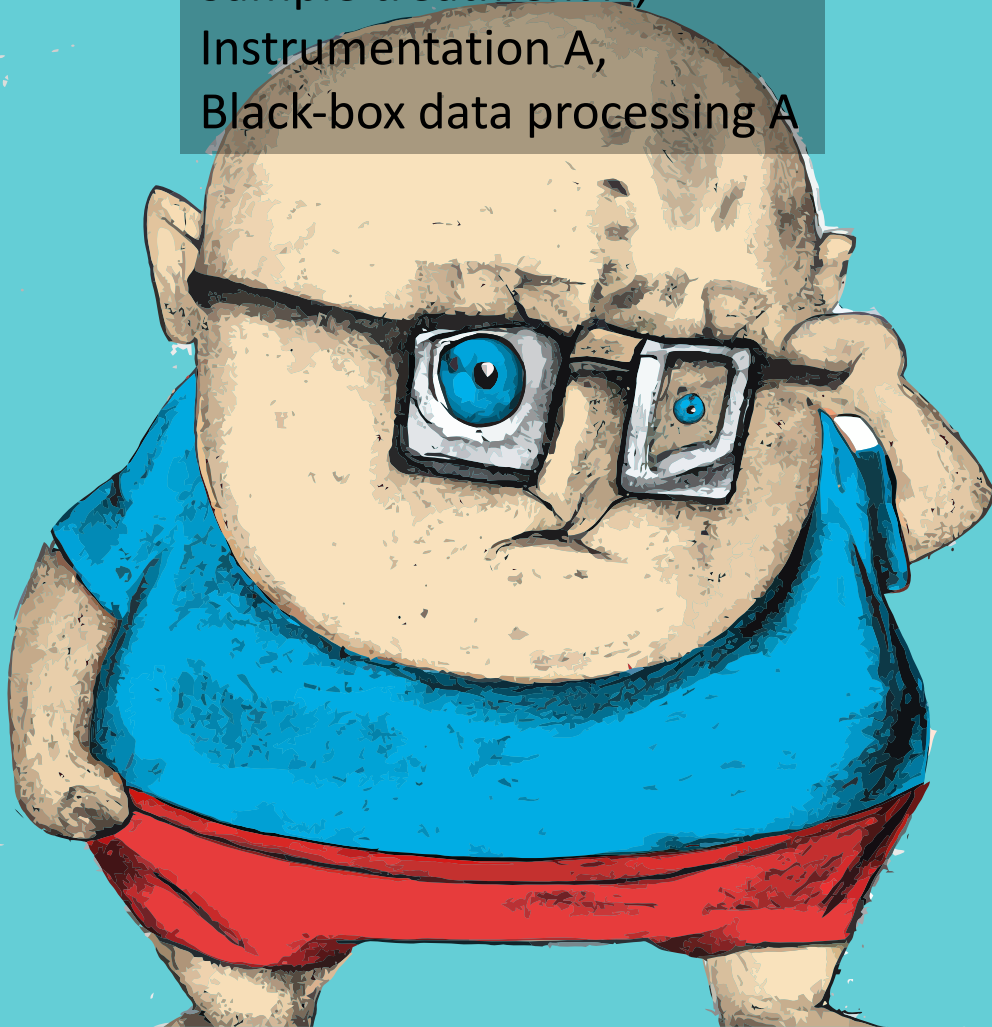


- Mass per NP
↳ size
- C_{number}
- C_{mass}

TRUENESS?

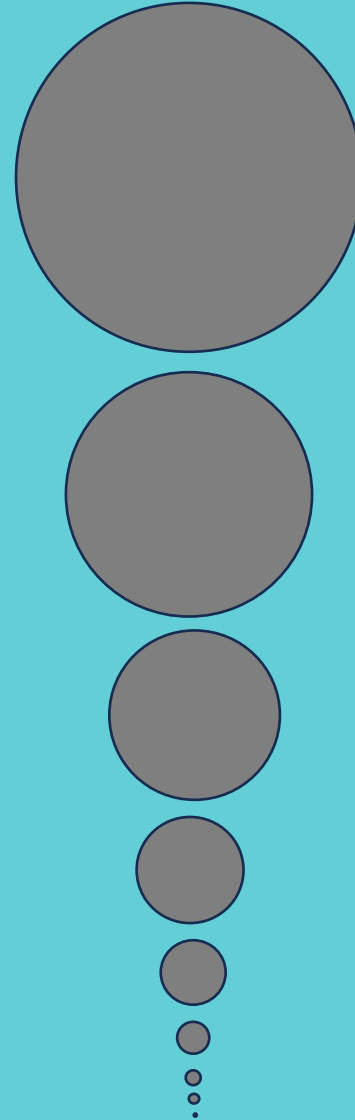
Lab A

Sample treatment A,
Instrumentation A,
Black-box data processing A



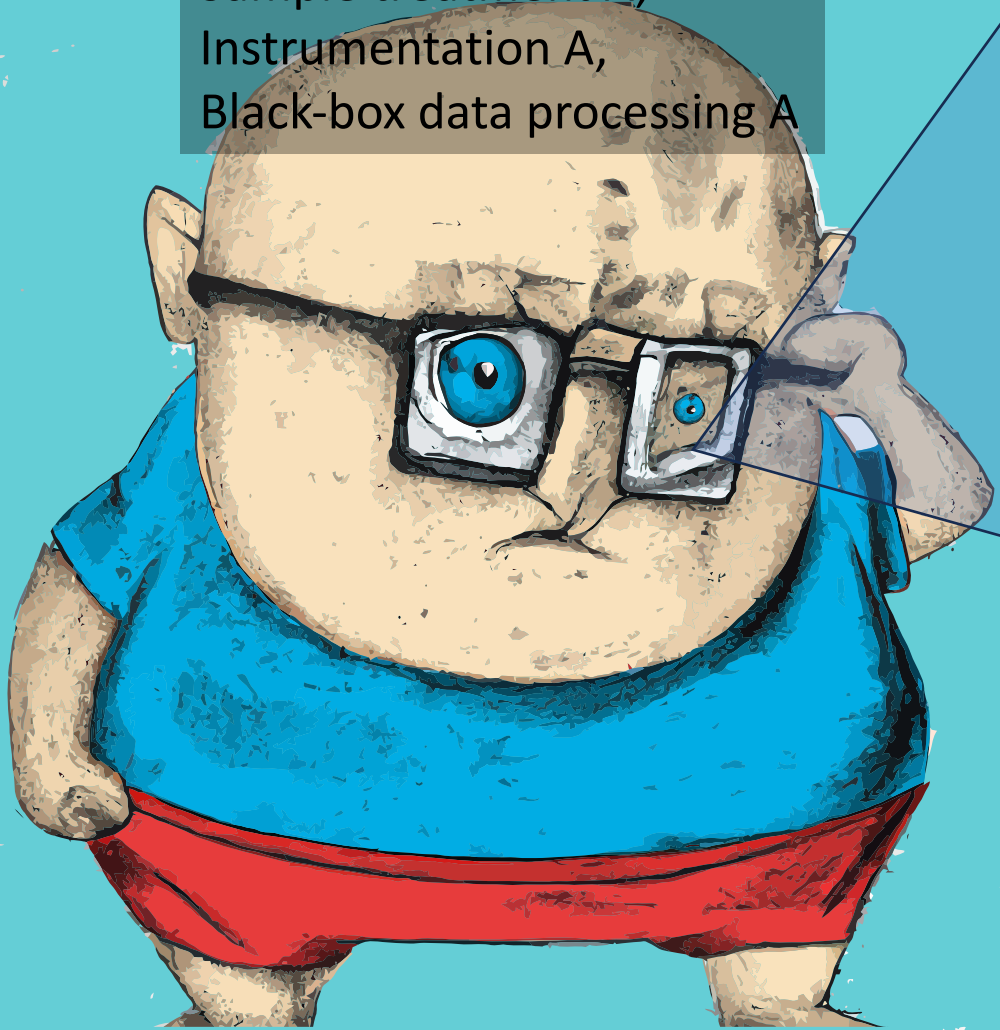
Lab B

Sample treatment B,
Instrumentation B,
Black-box data processing B



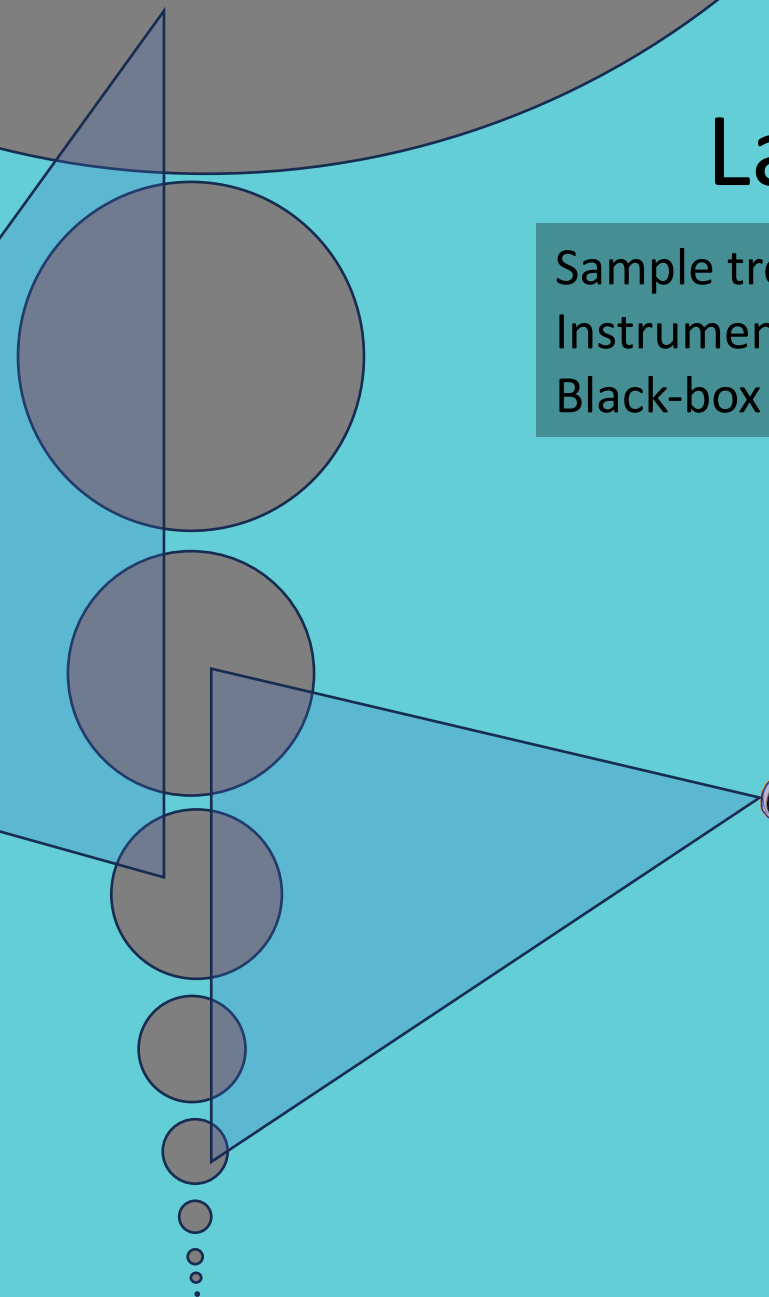
Lab A

Sample treatment A,
Instrumentation A,
Black-box data processing A



Lab B

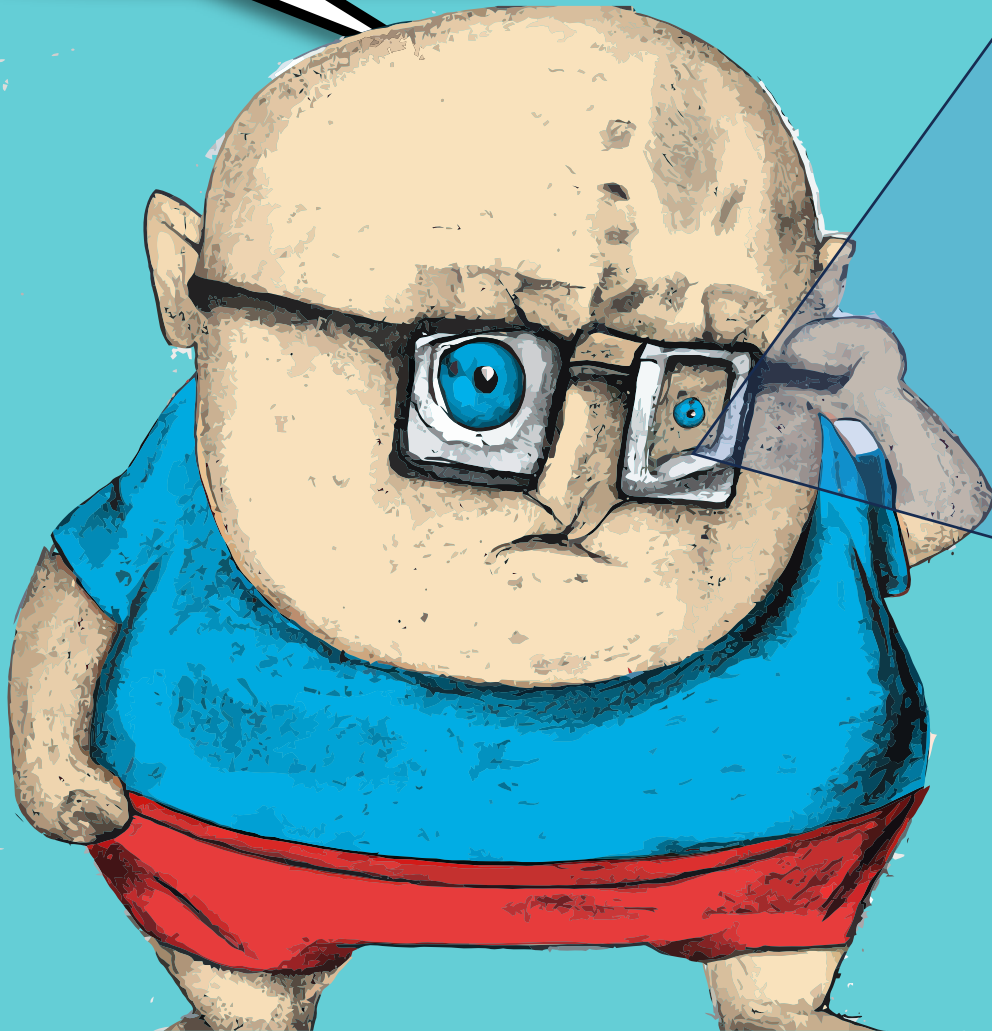
Sample treatment B,
Instrumentation B,
Black-box data processing B



800 ng/L.
 10^9 particles/L.
Median diameter 200 nm.

$\alpha ?$ $\beta ?$

No. 50 ng/L.
 10^{11} particles/L.
Median diameter 50 nm!



800 ng/L.
 10^9 particles/L.
Median diameter 200 nm.

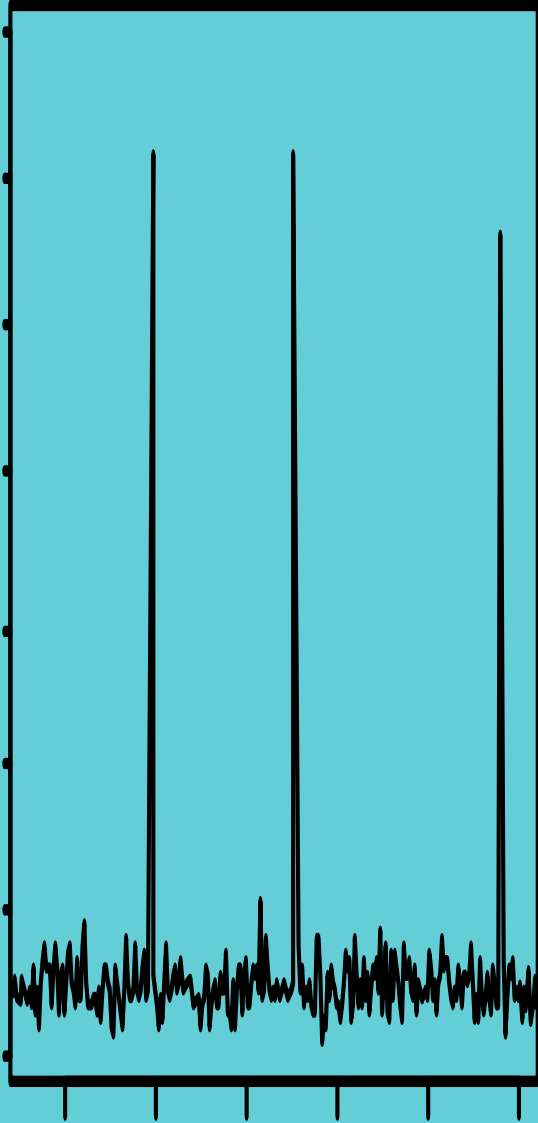


No. 50 ng/L.
 10^{11} particles/L.
Median diameter 50 nm!



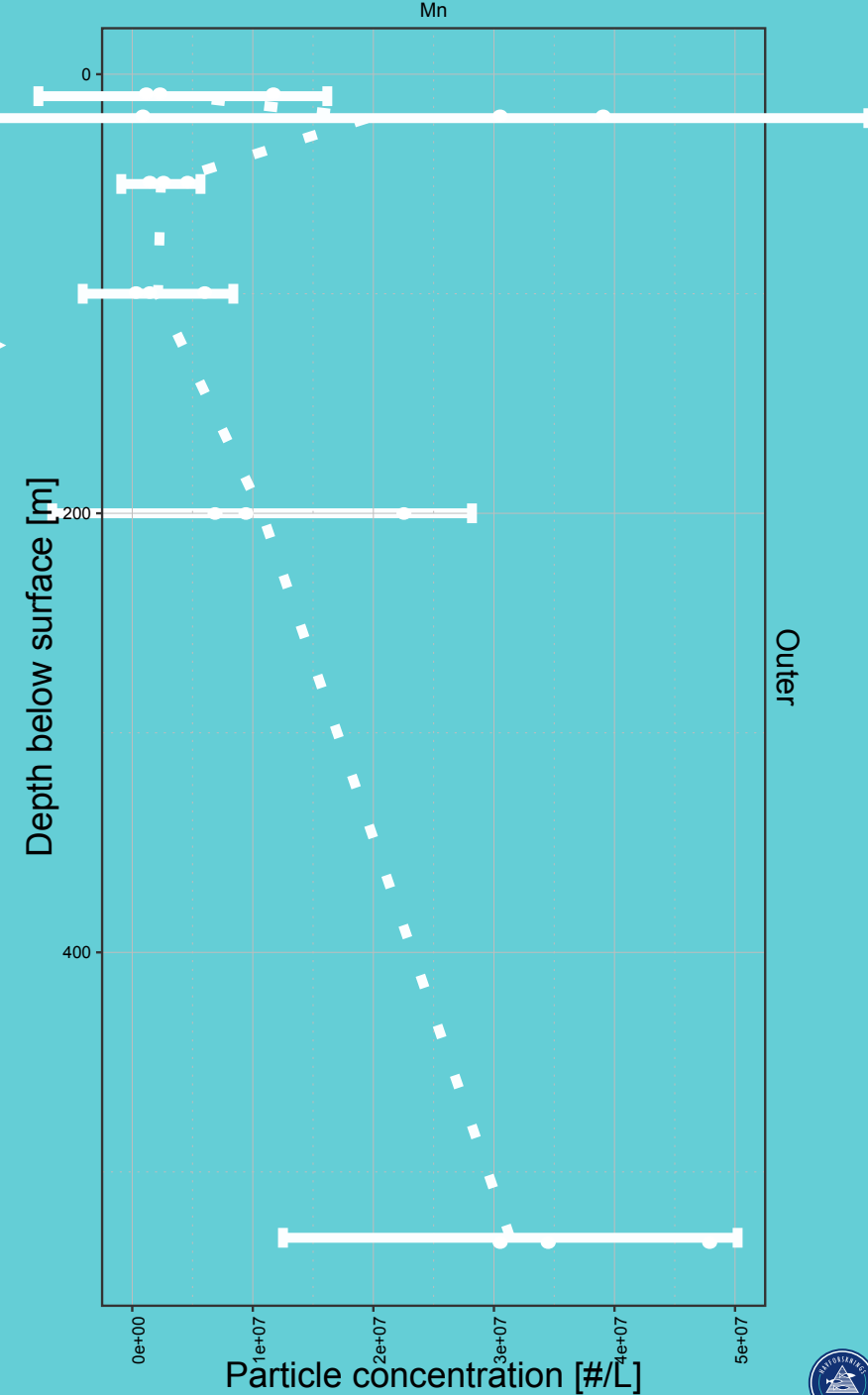
«OPERATIONALLY (UN)DEFINED METHOD»

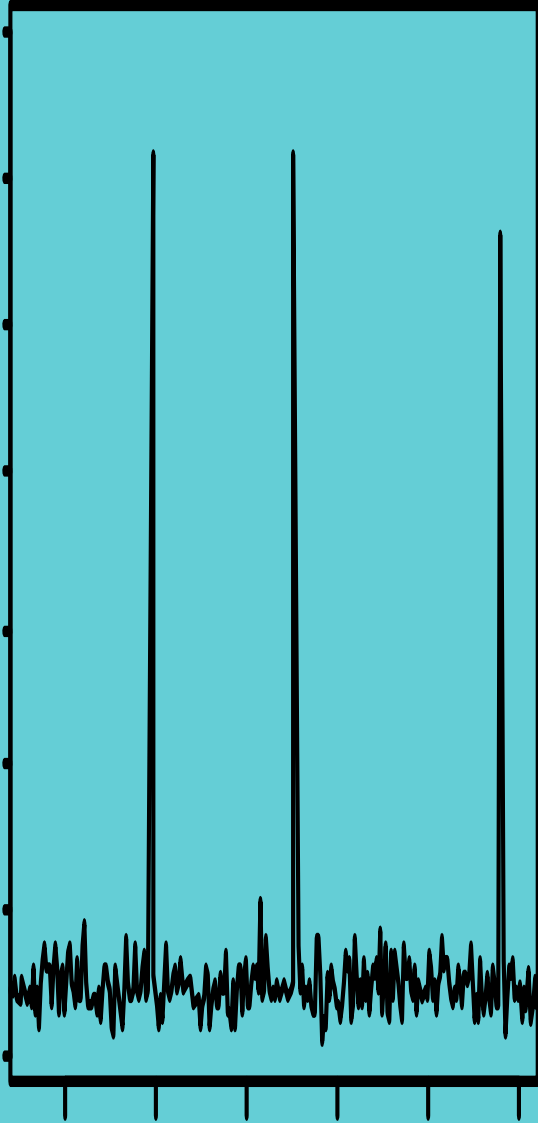




COMMERCIAL
SOFTWARE ©

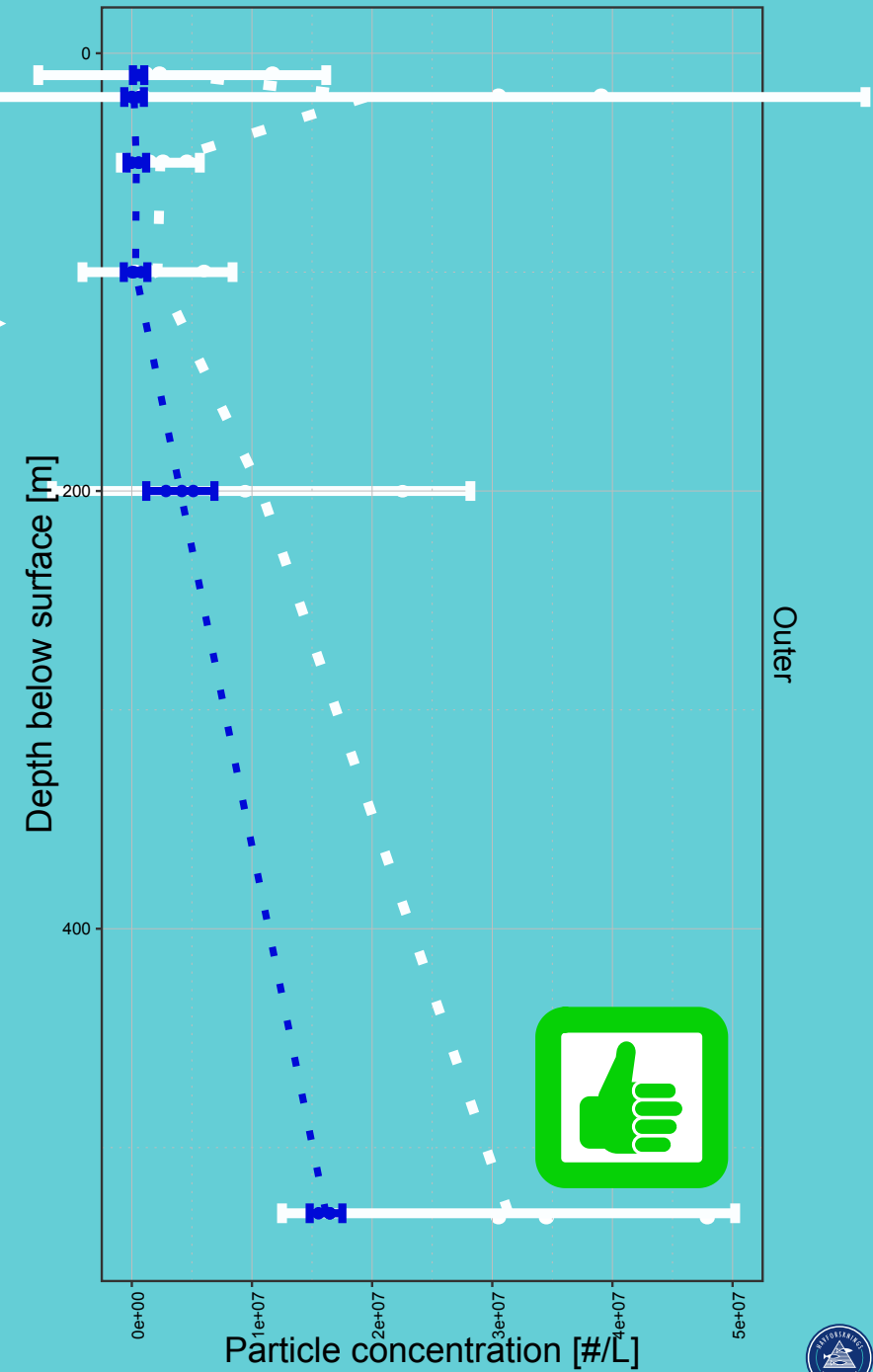
- Untransparent/black-box algorithm
- Detection limits not statistically defined
- Poor precision
- Manual work required





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SOFTWARE ©

- Open source
- α/β using Poisson statistics
- Improved precision
- Automated







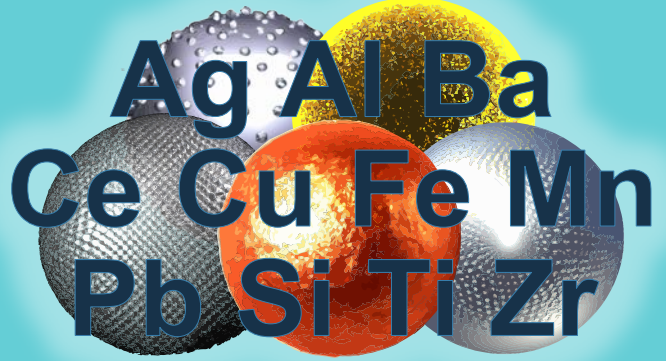
● Anthropogenic ● Farm ● Natural



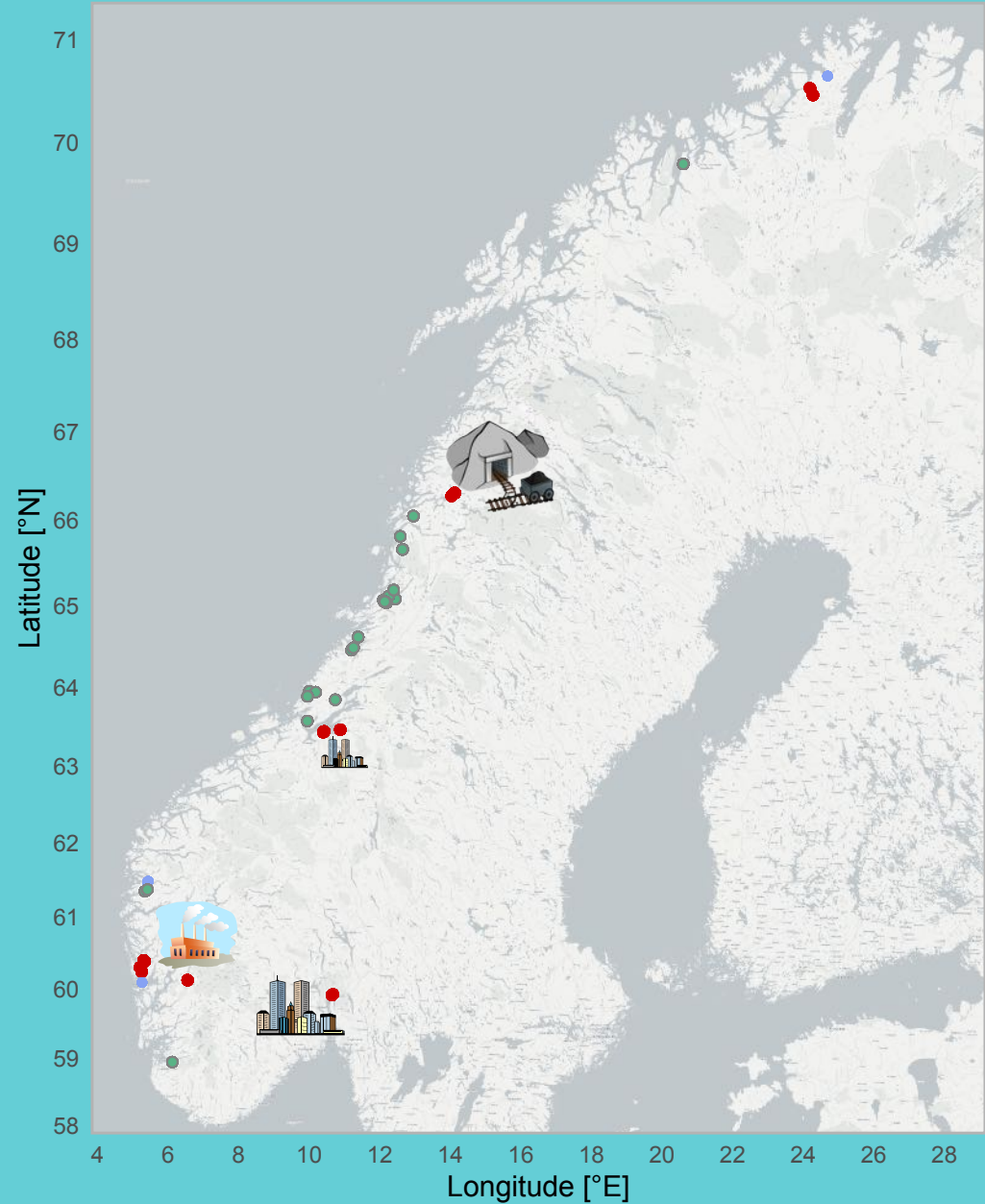
Determination of nanoparticles and metals in blue mussels along the Norwegian coastline



69 pooled samples

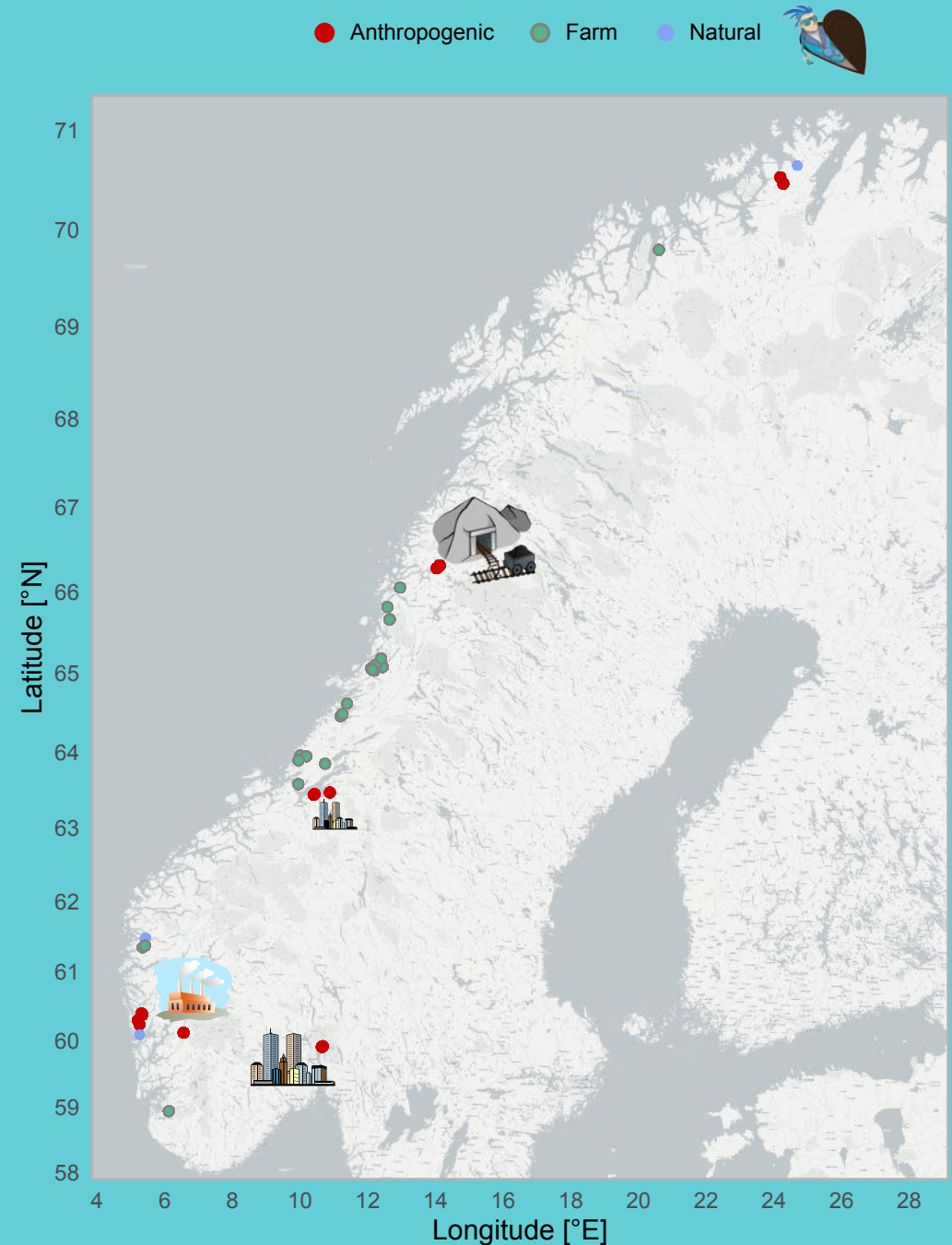
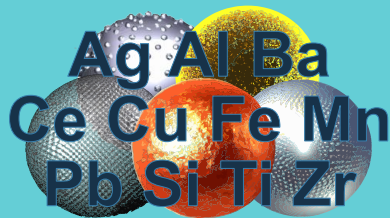


11 elements



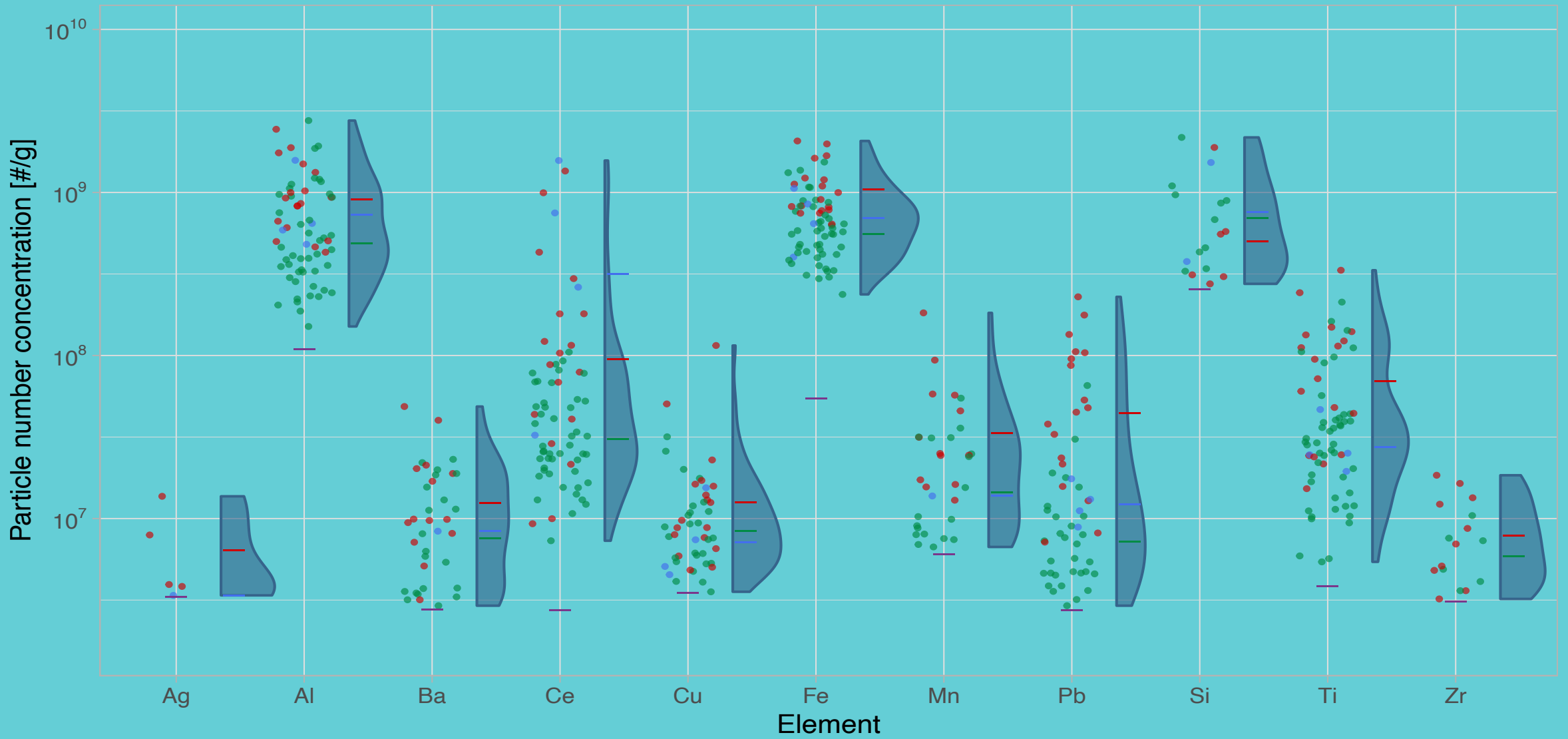
Determination of nanoparticles and metals in blue mussels along the Norwegian coastline

Levels and fractions of NPs vs metals?
Anthropogenic vs “pristine” locations?
Seasonality and mussel length as proxy for age

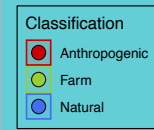
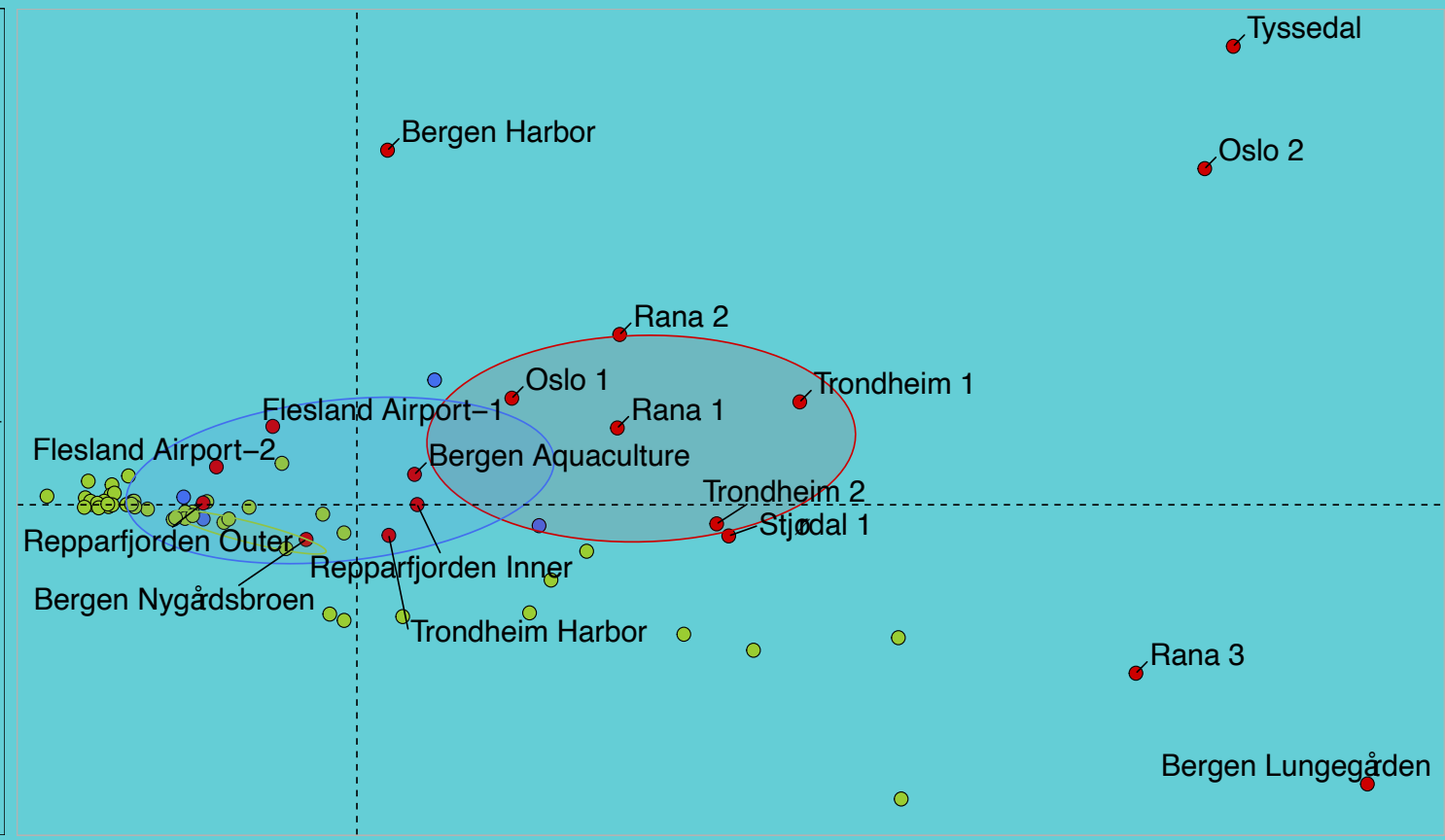
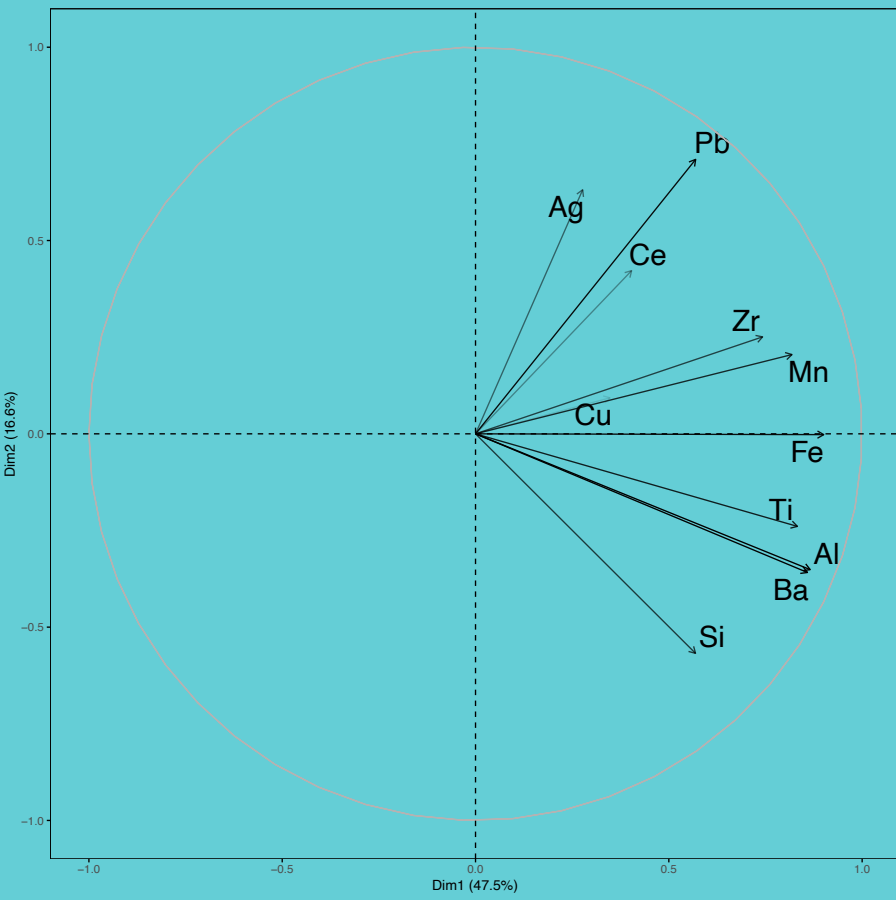


Levels of NPs

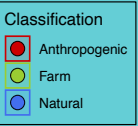
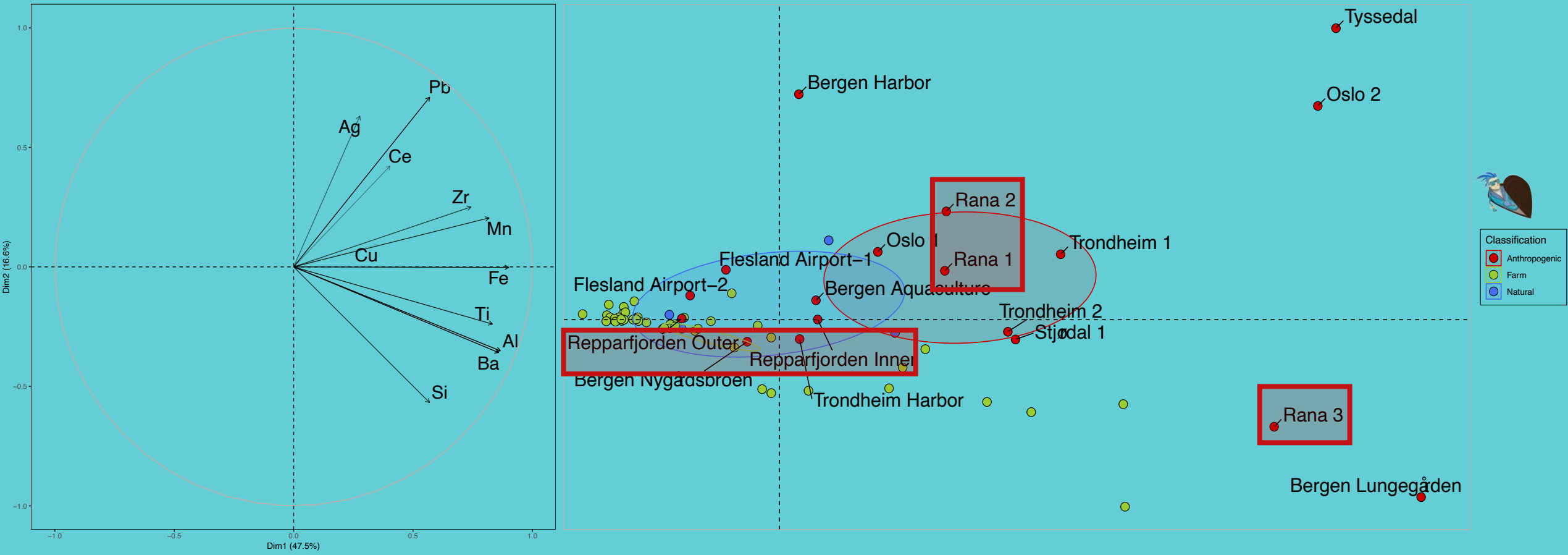
Anthropogenic Farm Natural 



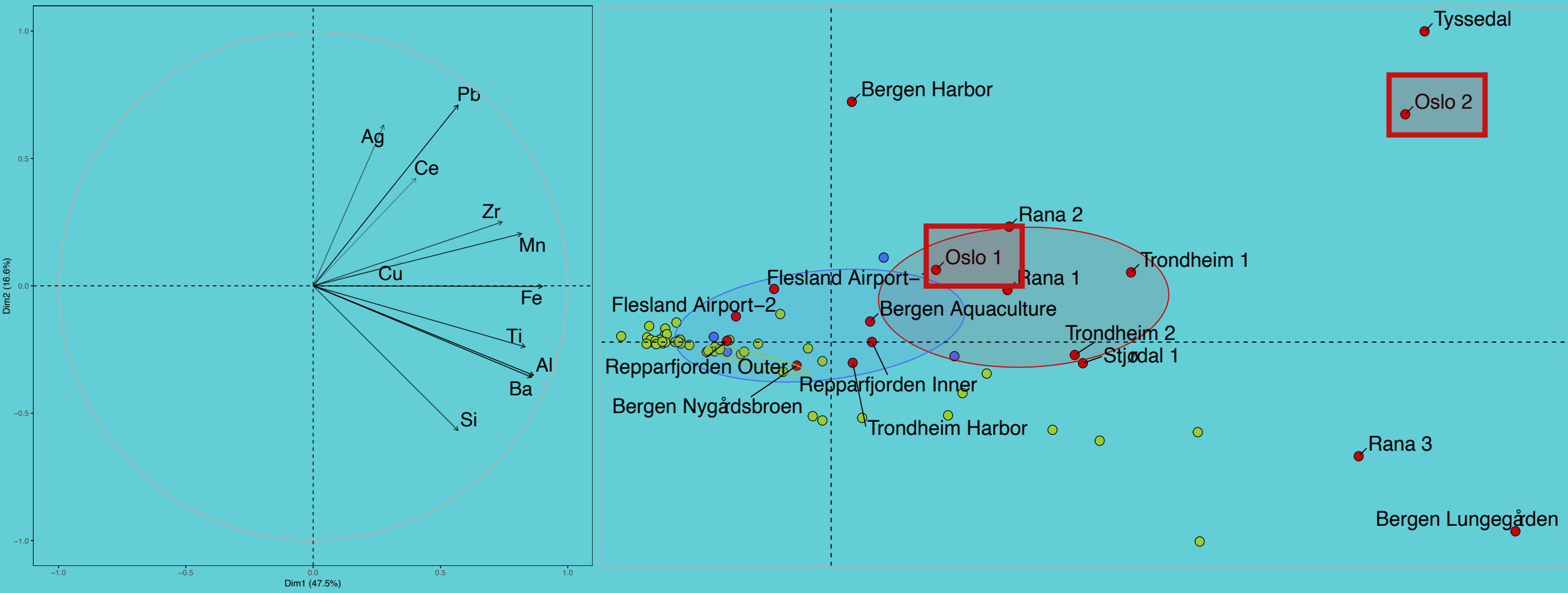
PCA



PCA



PCA

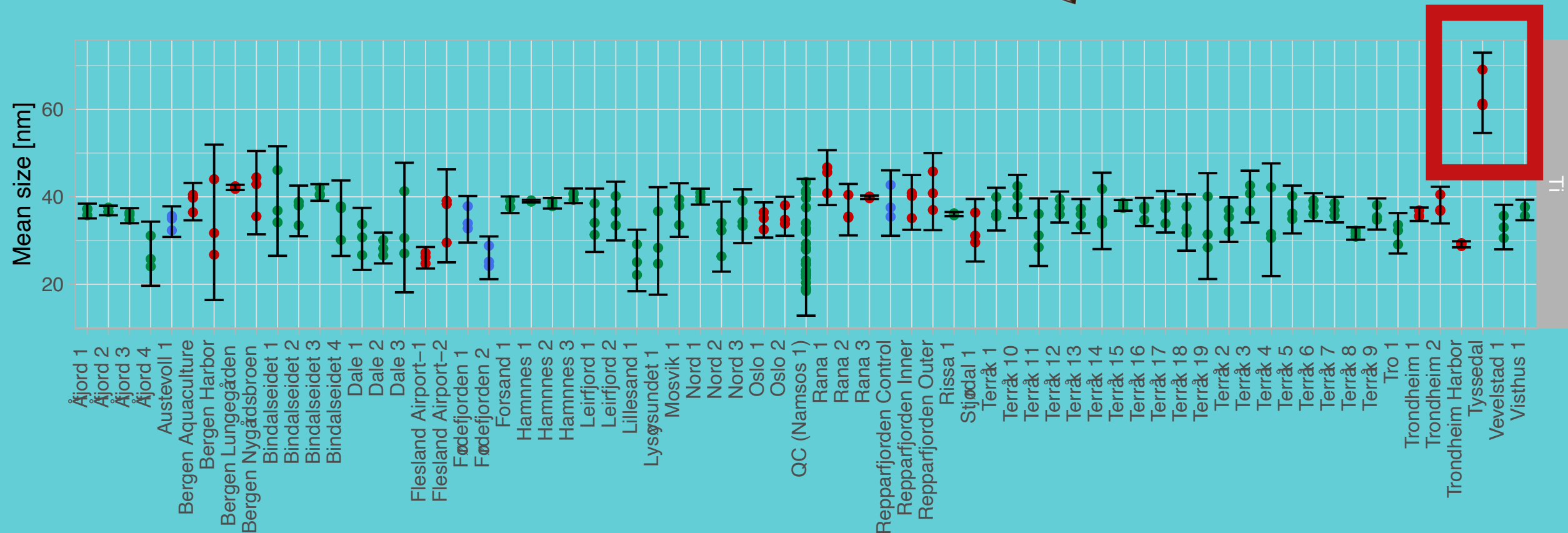


Classification

- Anthropogenic
- Farm
- Natural

Particle size (diameter)

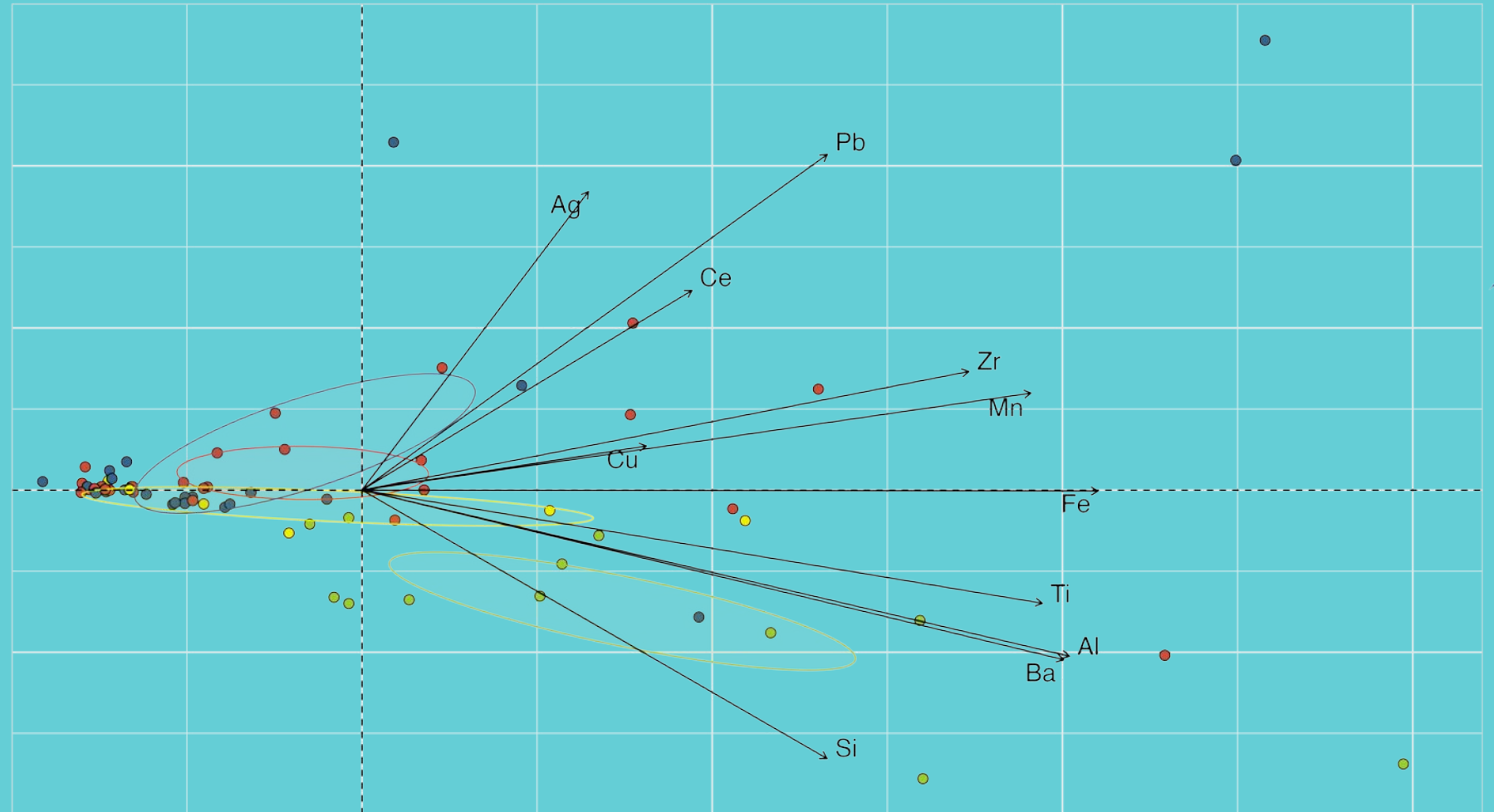
● Anthropogenic ● Farm ● Natural



Other factors

Confounders:

- Seasonality
- Shell length(?)



Seasonality

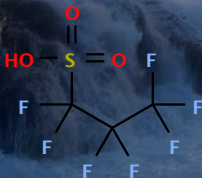
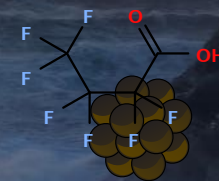
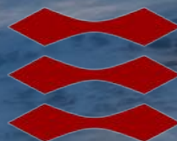
- Autumn
- Spring
- Summer
- Winter



Thanks!

also to Stig Valdersnes, Katrin Löschner, Monica Sanden

DTU



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