Data-driven modeling of nano-nose gas sensor arrays

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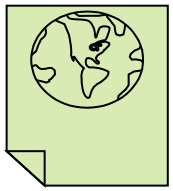
[a]Department of Informatics and Mathematical Modelling - DTU
[b]Department of Micro- and Nanotechnology - DTU
[c]Department of Chemistry – Univ. of Copenhagen

Xsense



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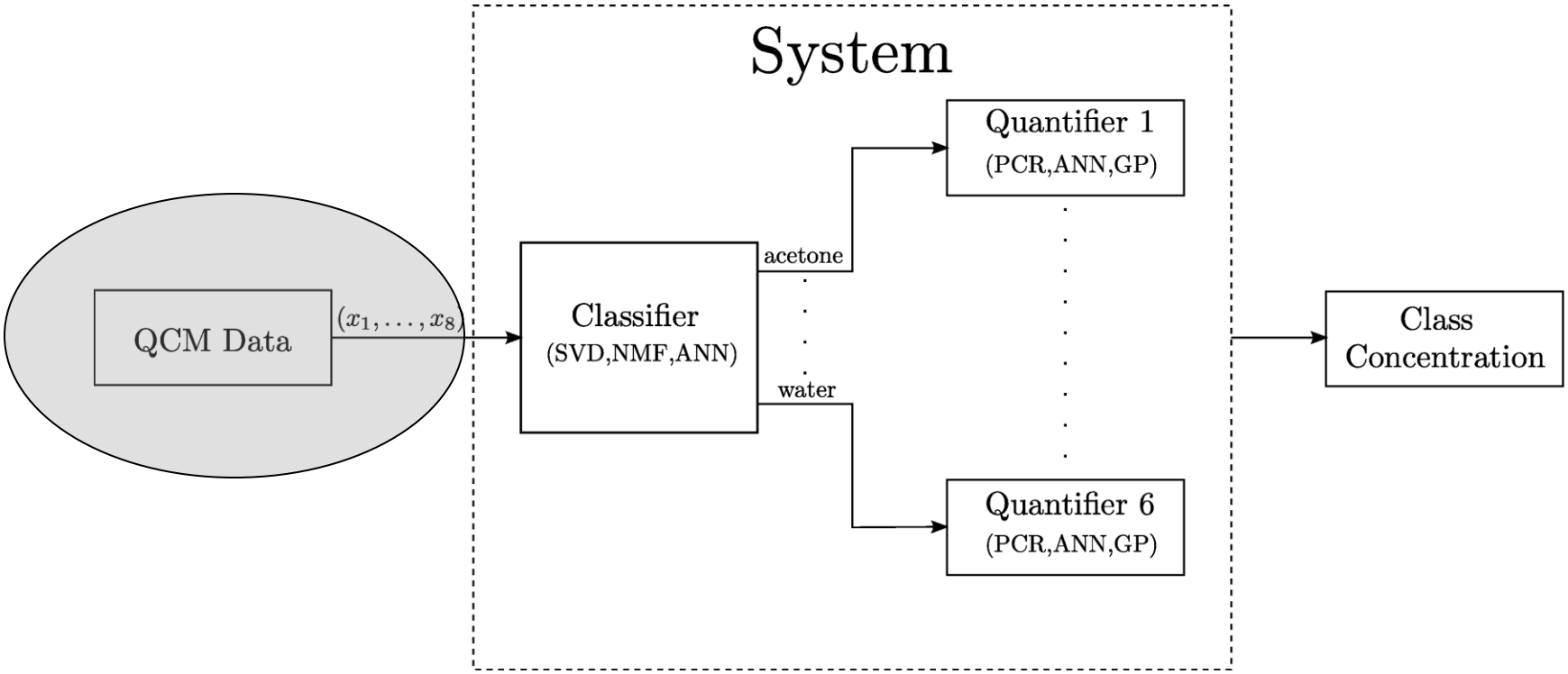
Department of Informatics and Mathematical Modeling

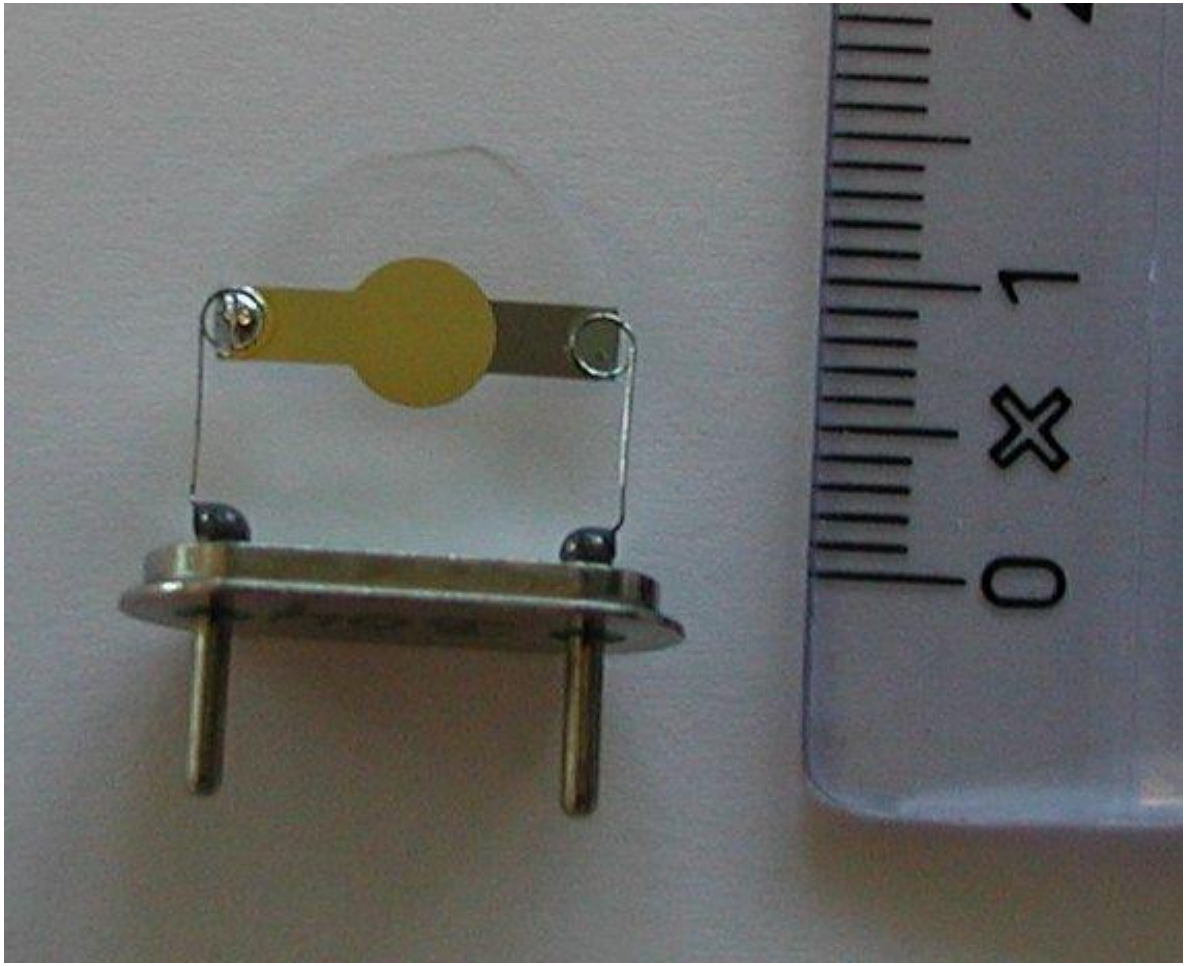
Introduction

- We present a gas sensor based on eight polymer coated quartz crystals using quartz crystal microbalance (QCM) as measuring technique
- The sensor is exposed to six different analytes at various concentration levels
- The analytes are classified using Singular Value Decomposition (SVD), Non-negative Matrix factorization (NMF) and Artificial Neural Networks (ANN)
- Analyte concentration level is estimated using Principal Component Regression (PCR), Neural Network Regression (NNR) and Gaussian Process Regression (GPR)
- Application areas could be drug control, border control, homeland security, anti terror activities, food control, environmental monitoring and medical technology

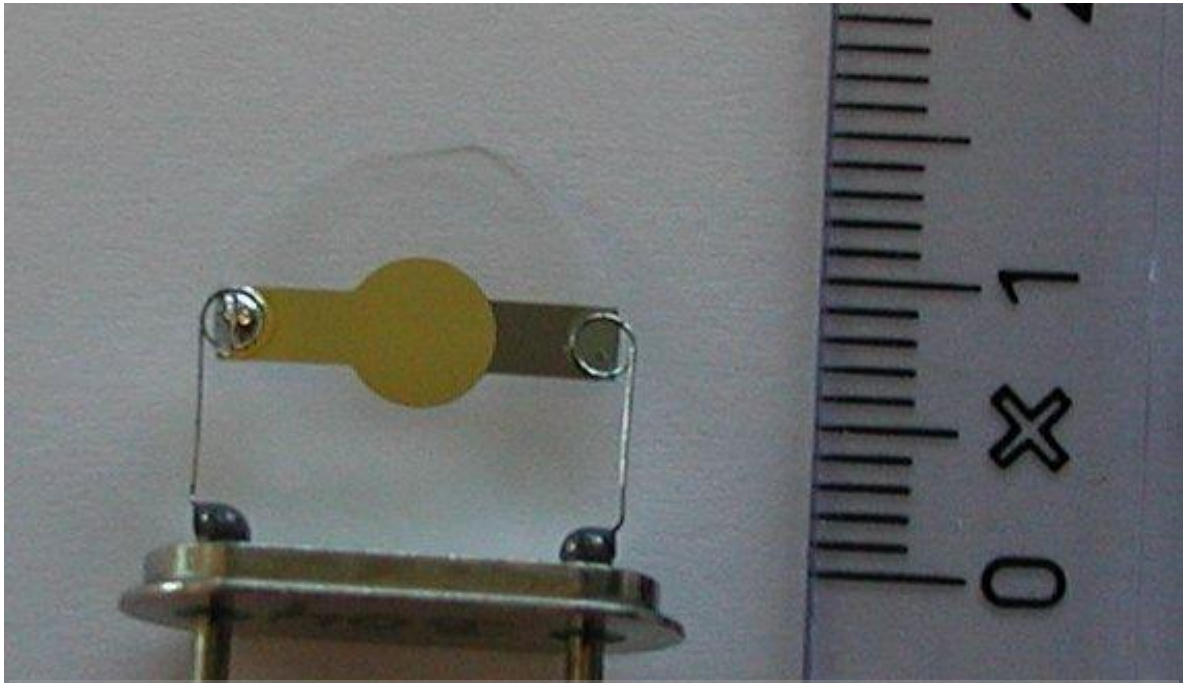
Data processing framework



Quartz Crystal Microbalance



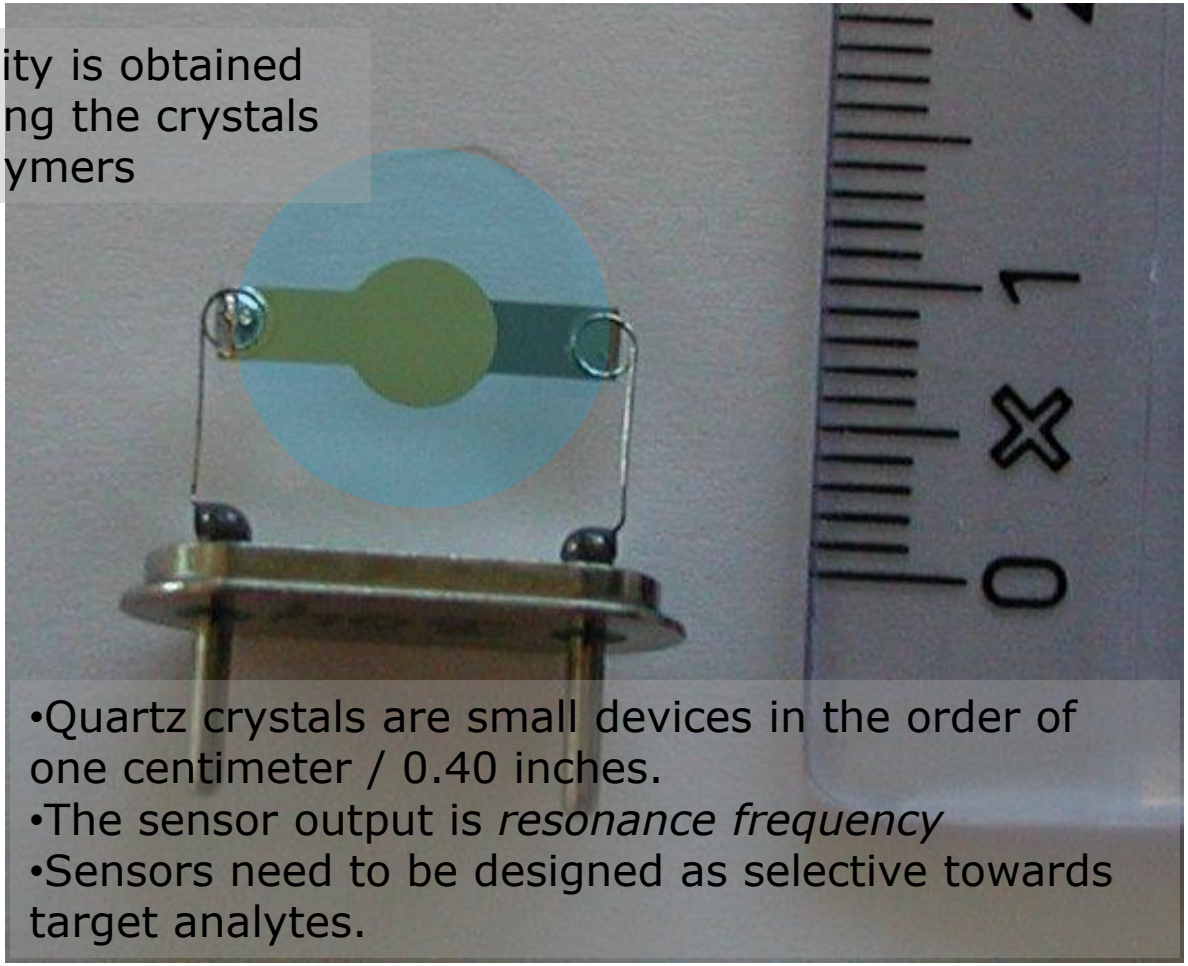
Quartz Crystal Microbalance



•Quartz crystals are small devices in the order of one centimeter / 0.40 inches.
•The sensor output is *resonance frequency*
•Sensors need to be designed as selective towards target analytes.

Quartz Crystal Microbalance

Selectivity is obtained by coating the crystals with polymers



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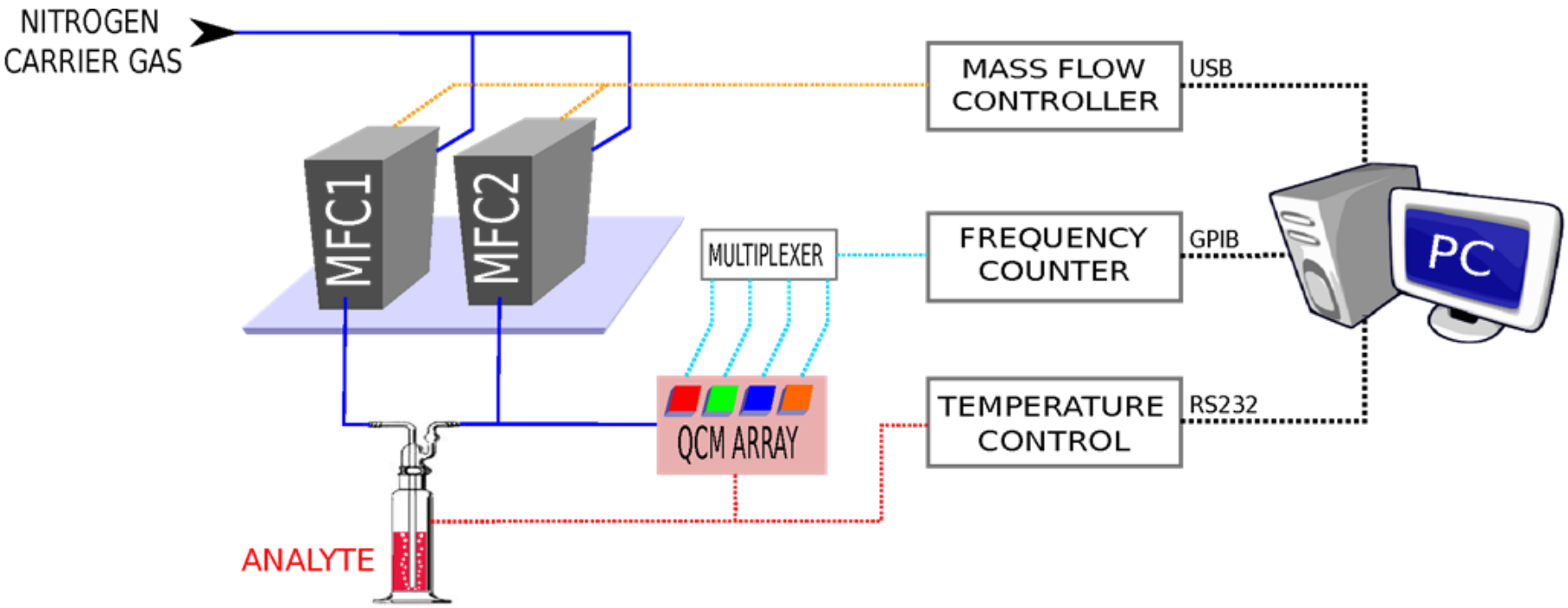
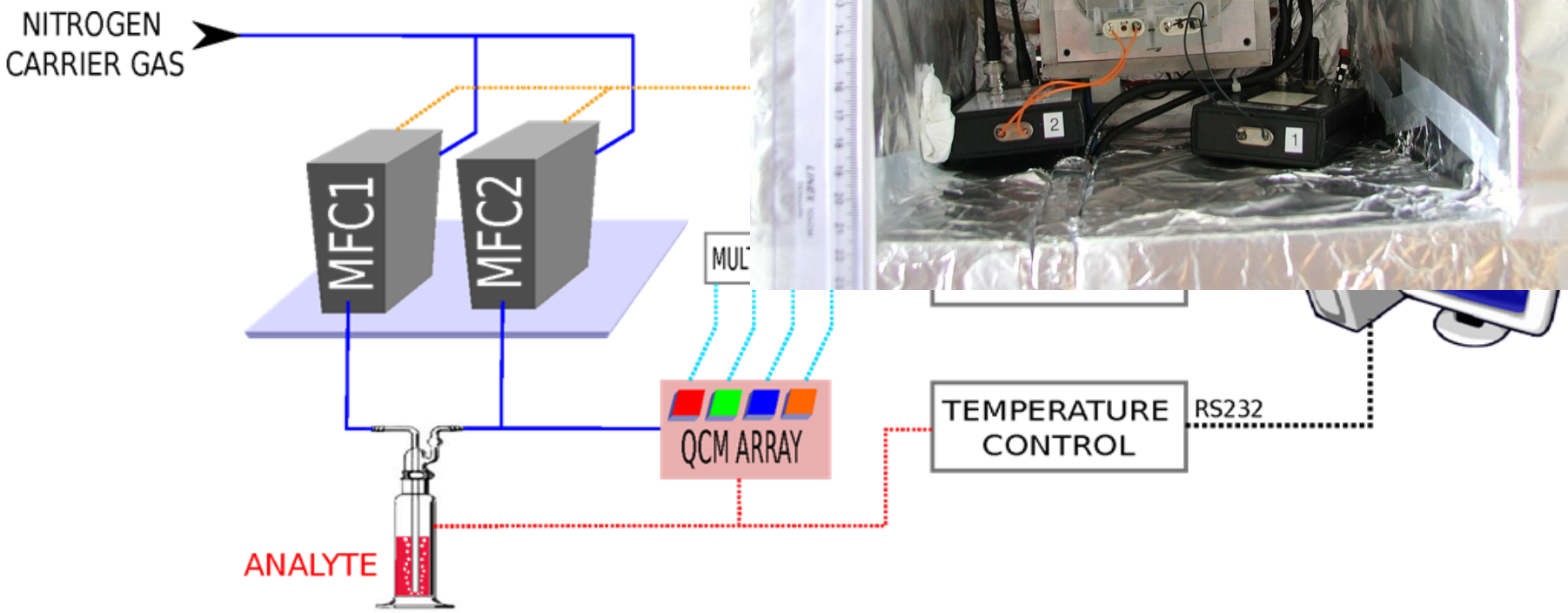
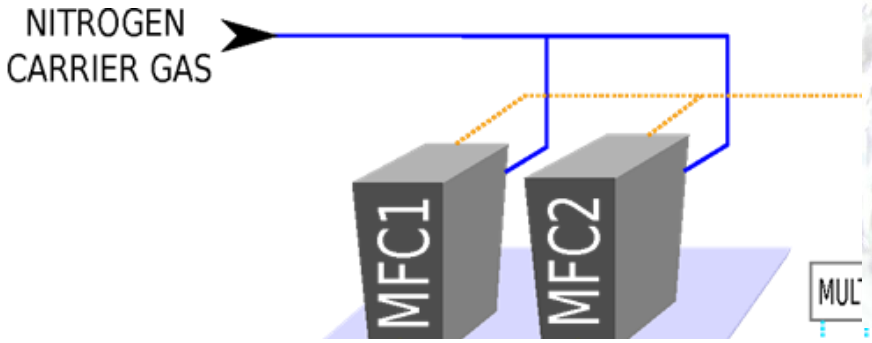
Flow Controller setup

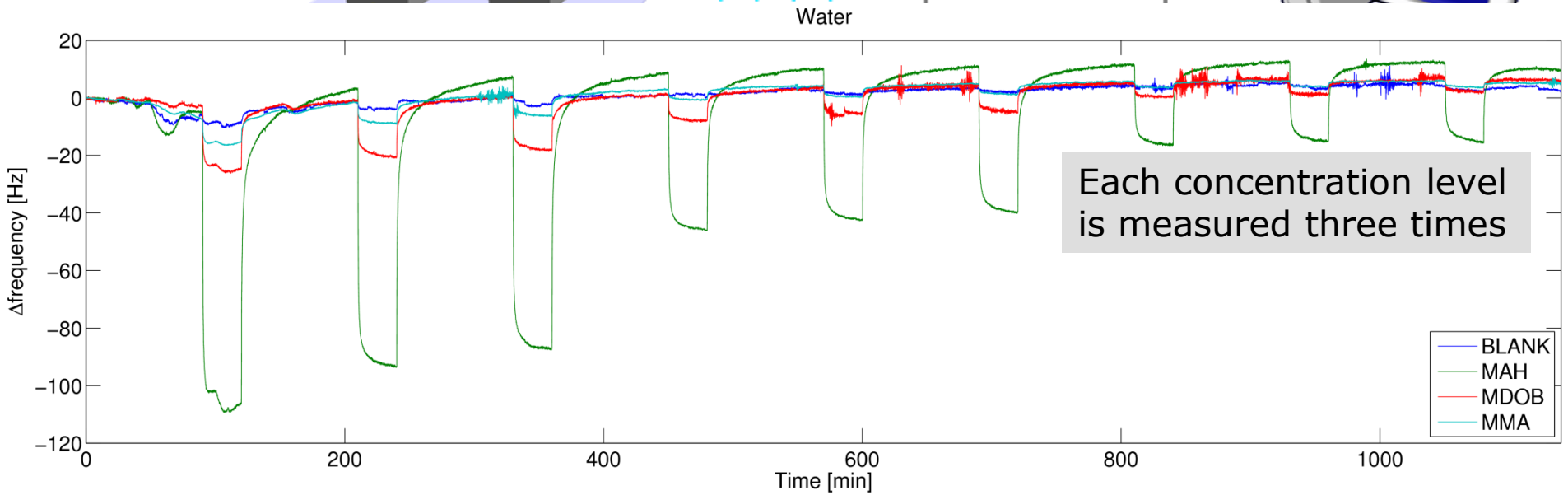


Flow Controller setup

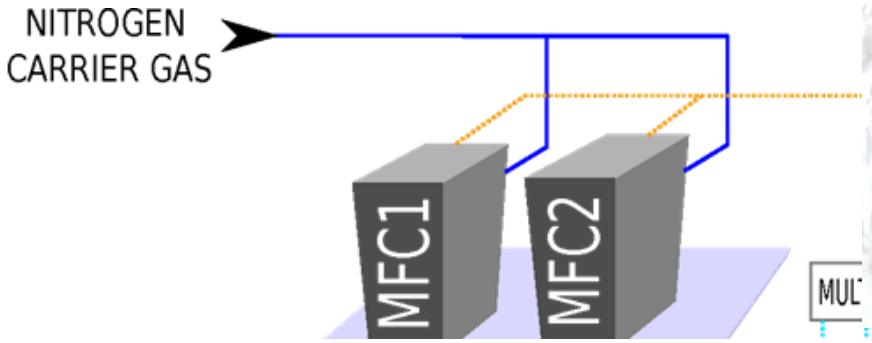


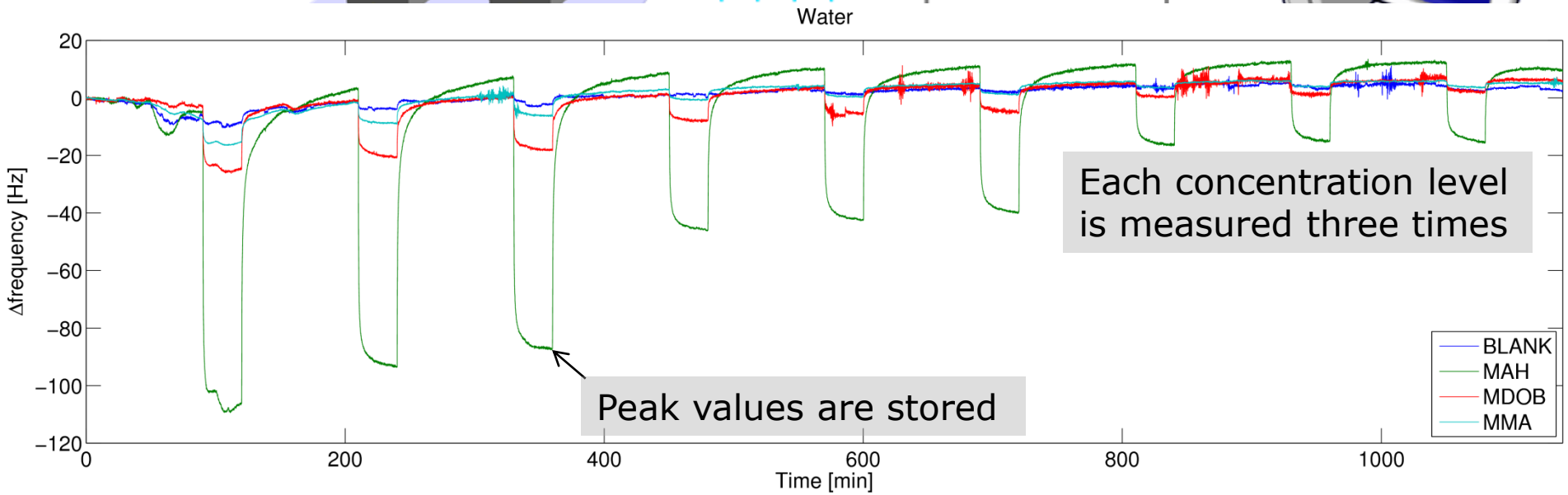
Flow Controller setup



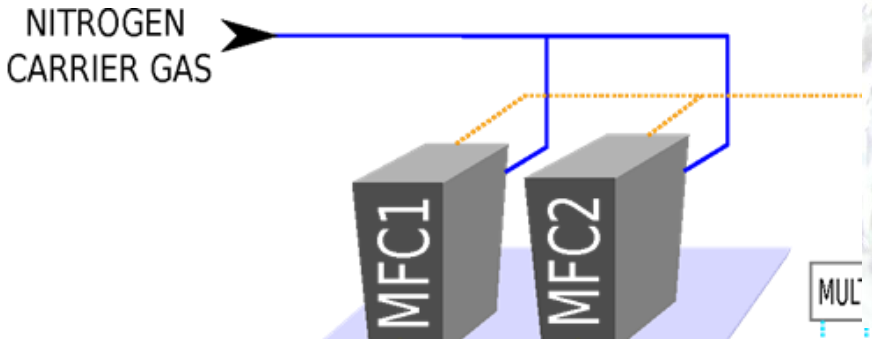


Flow Controller setup

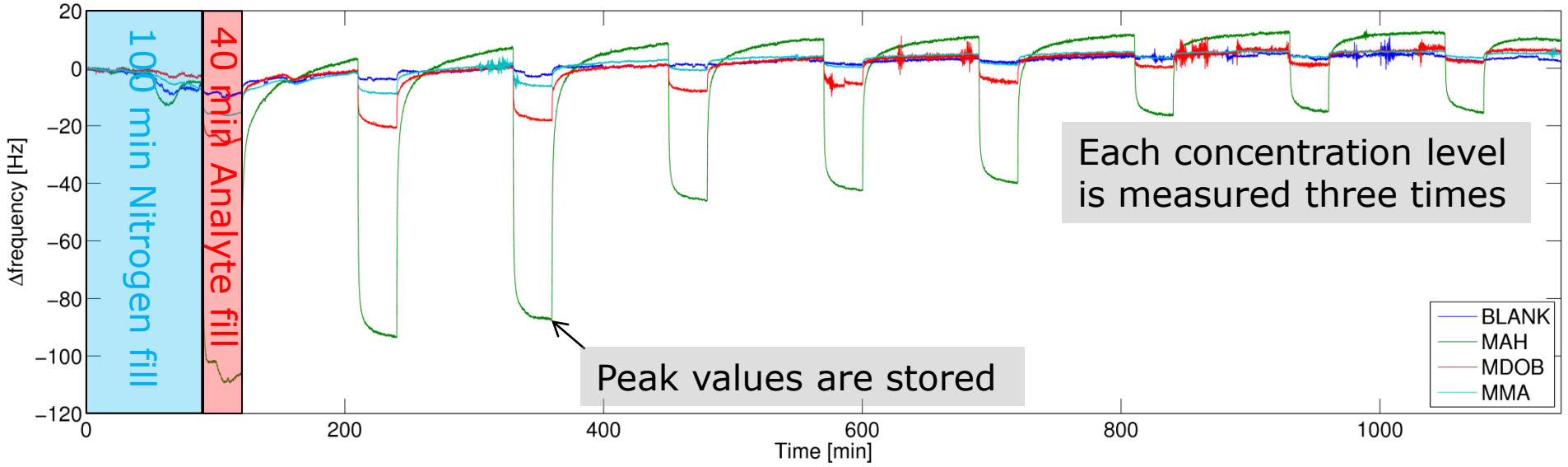




Flow Controller setup

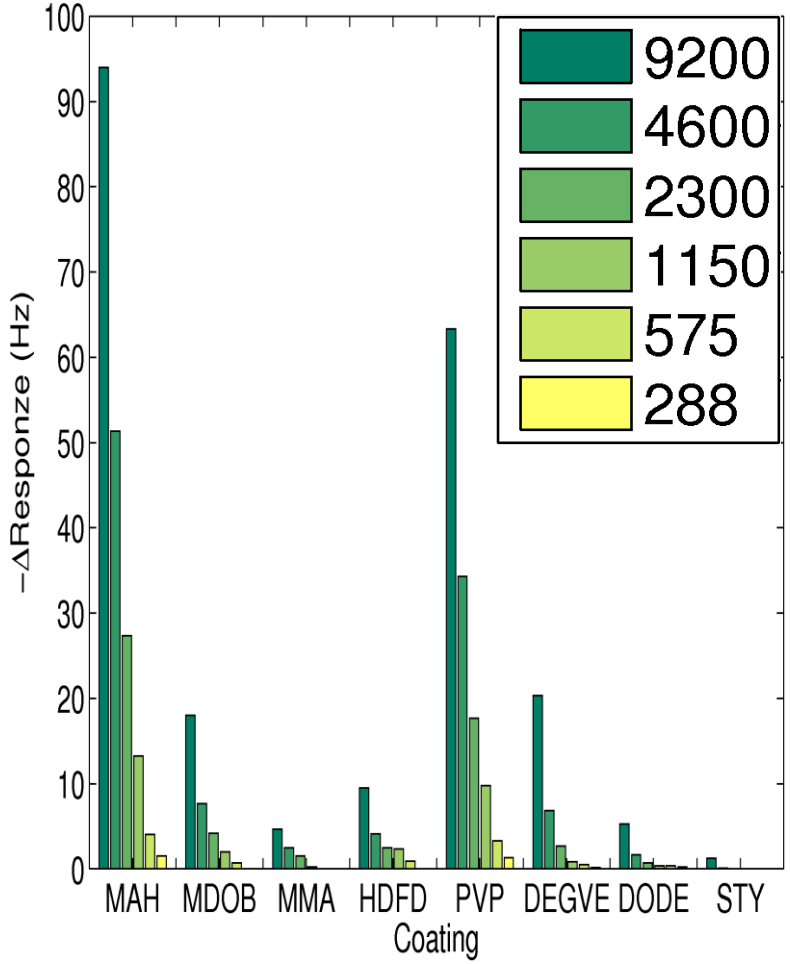


Water

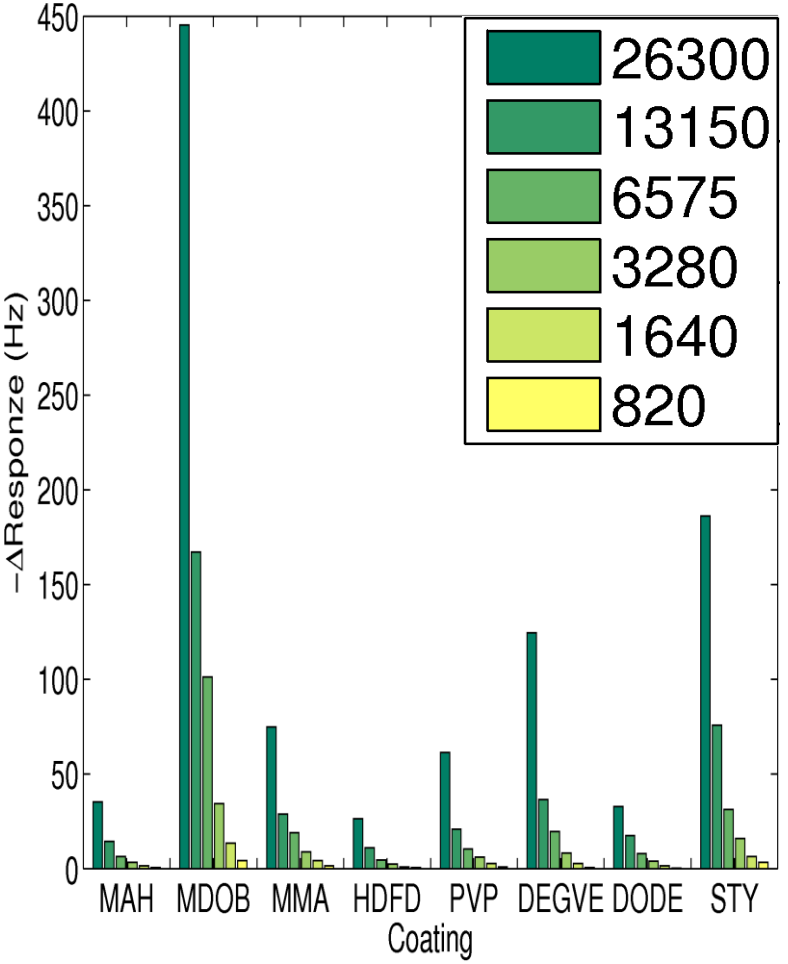


Frequency readings

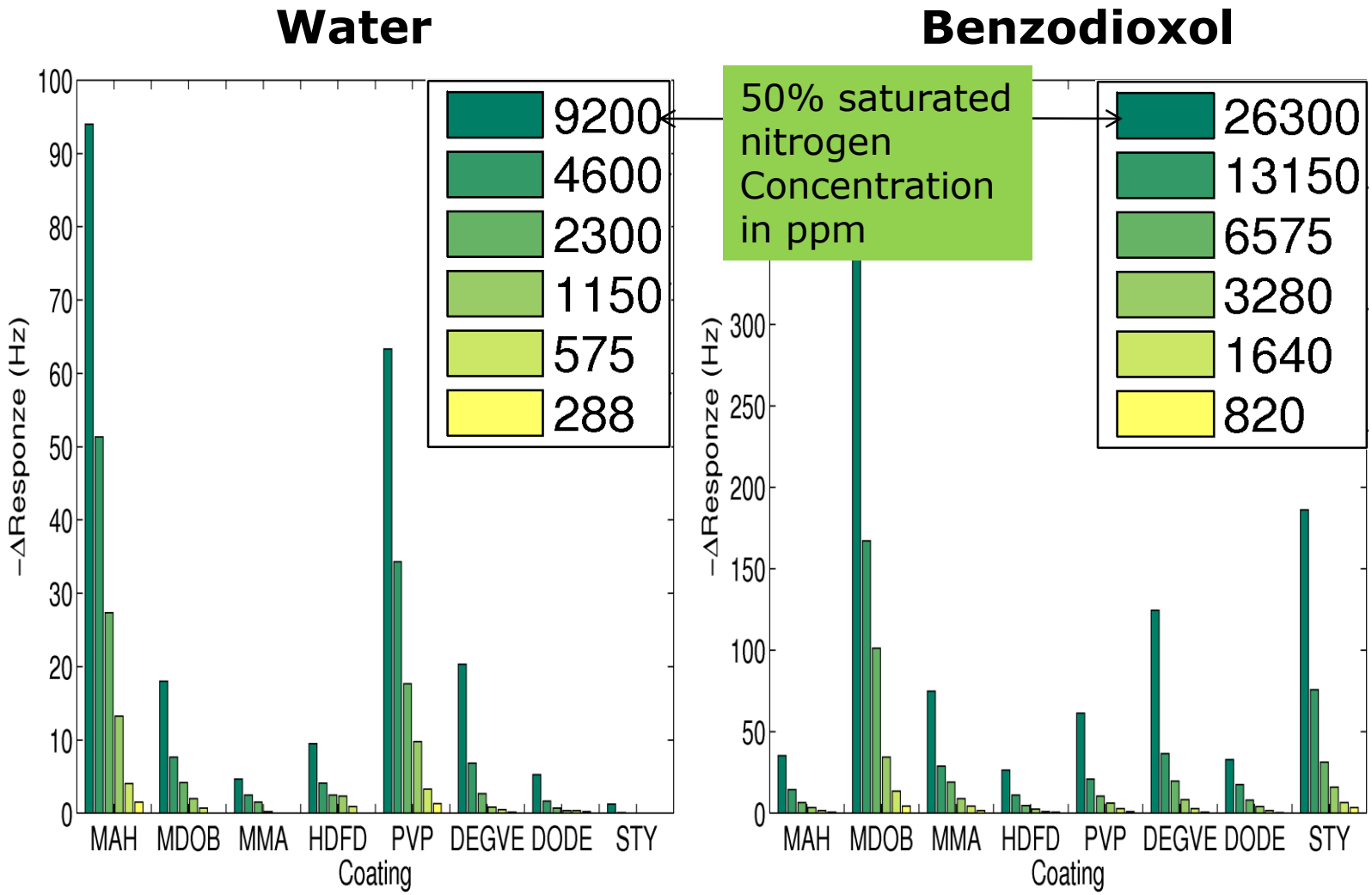
Water



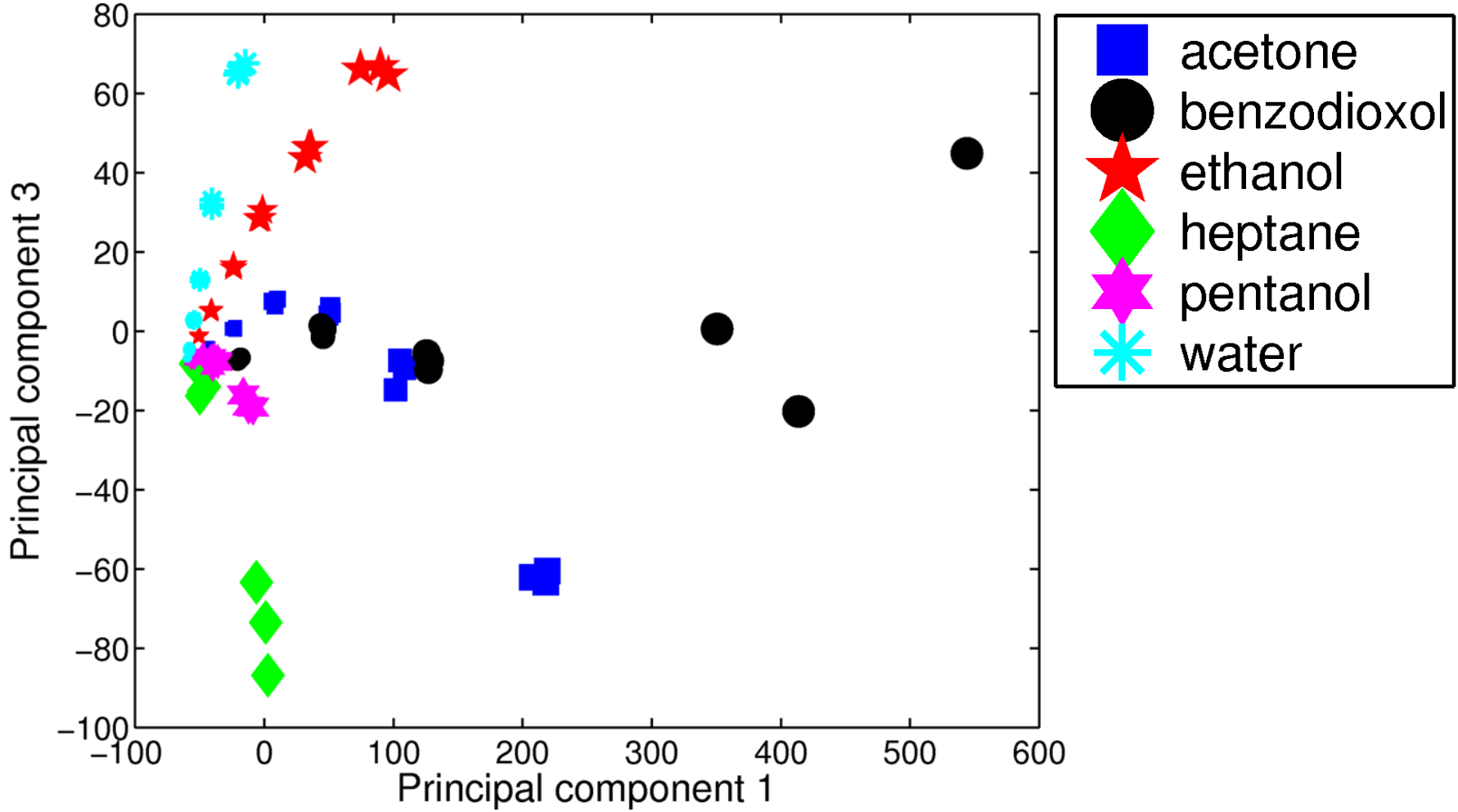
Benzodioxol



Frequency readings



Data is visualized using Principal Component Analysis (PCA)



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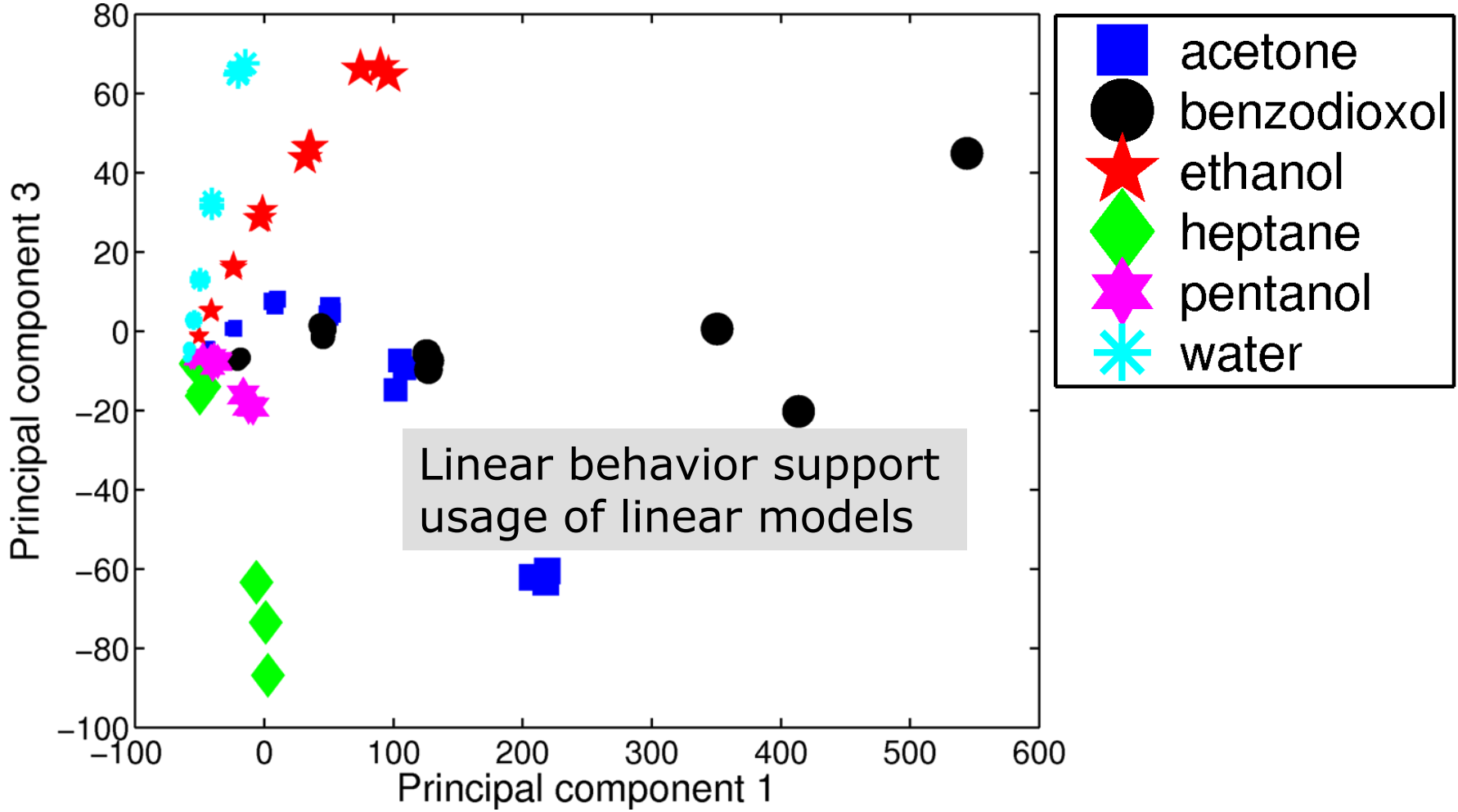

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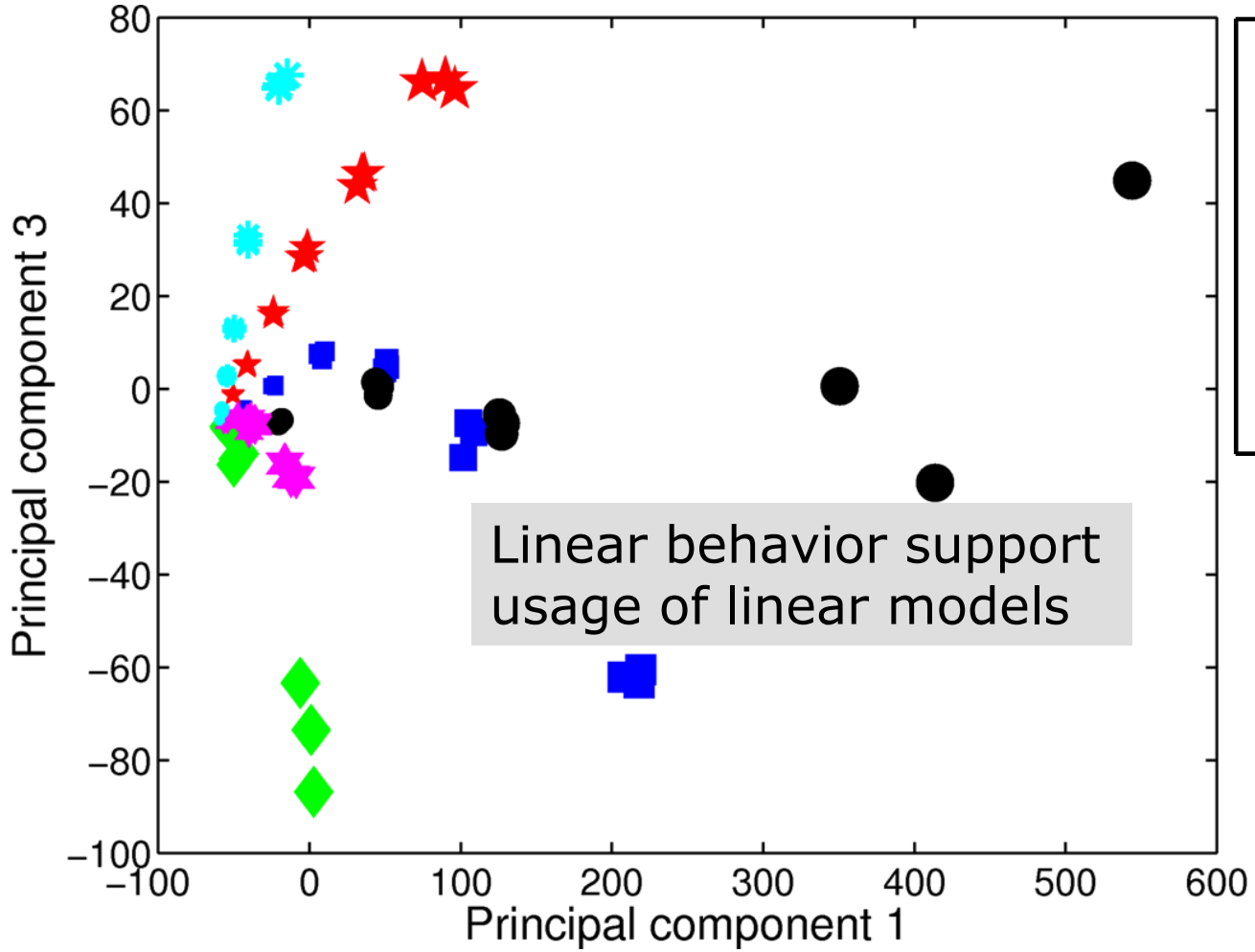
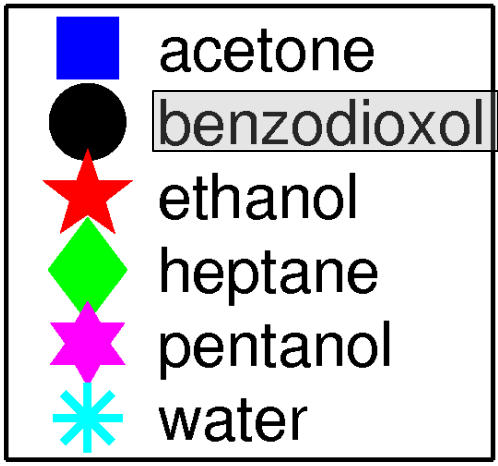
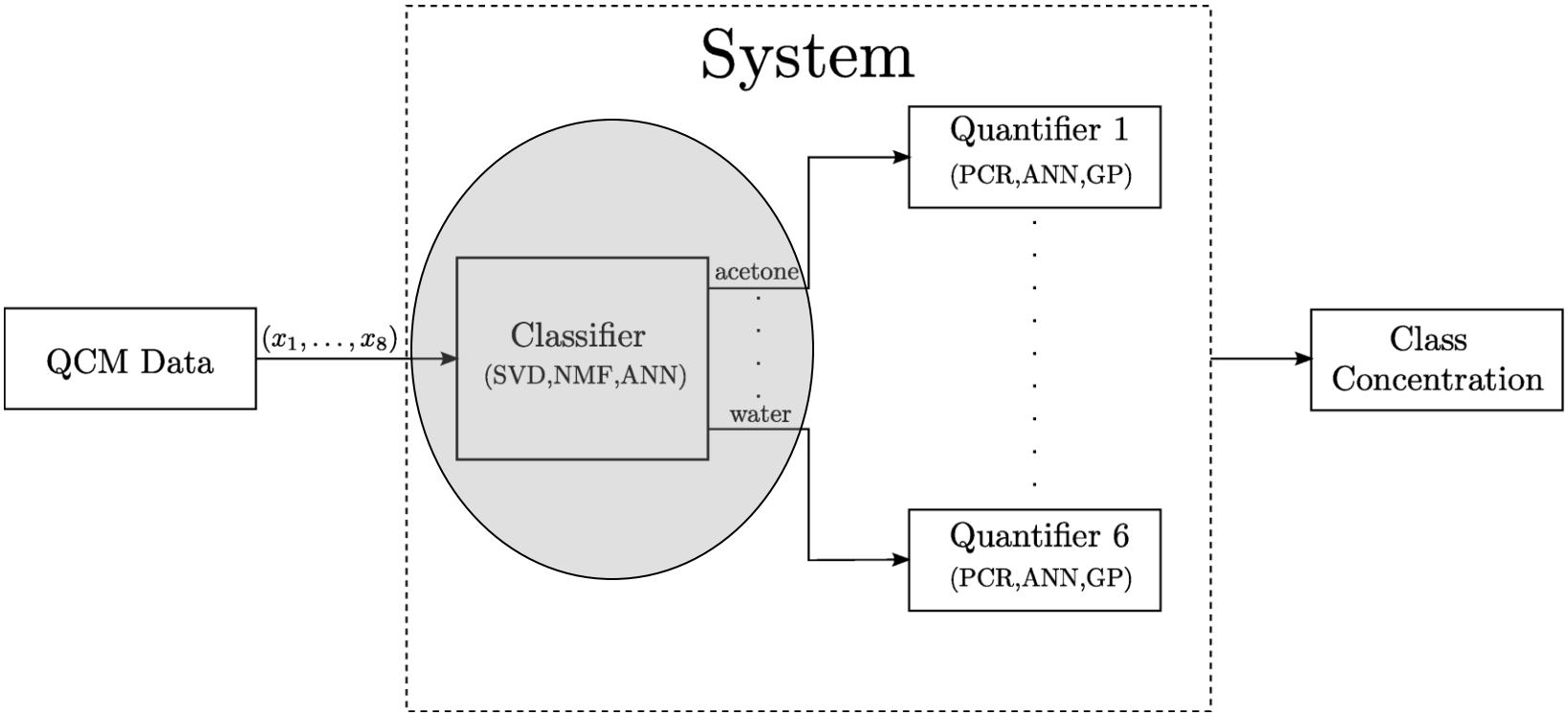


Linear behavior support usage of linear models

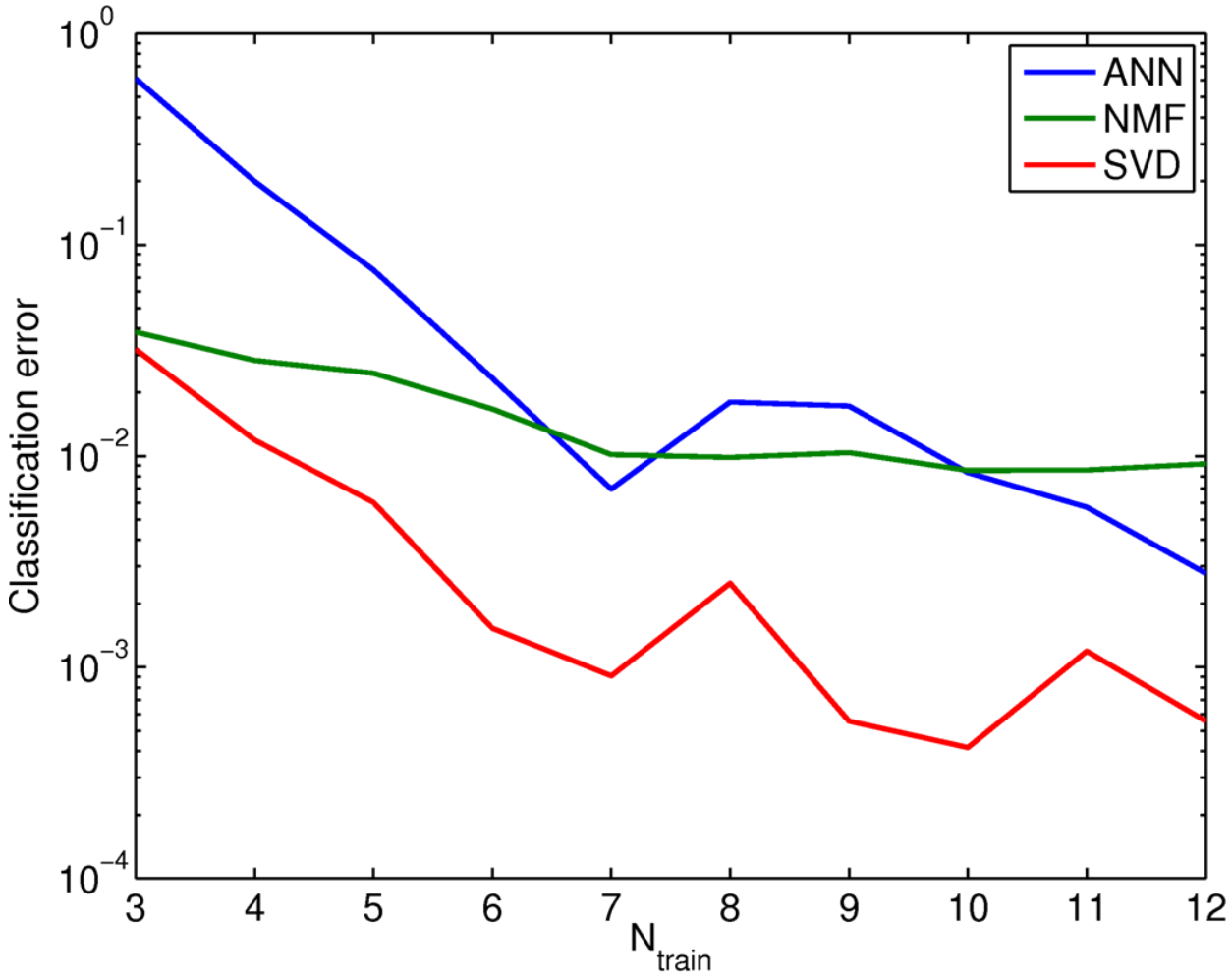


Precursor for Ecstacy

Data processing framework



Classification results – average over 100 runs



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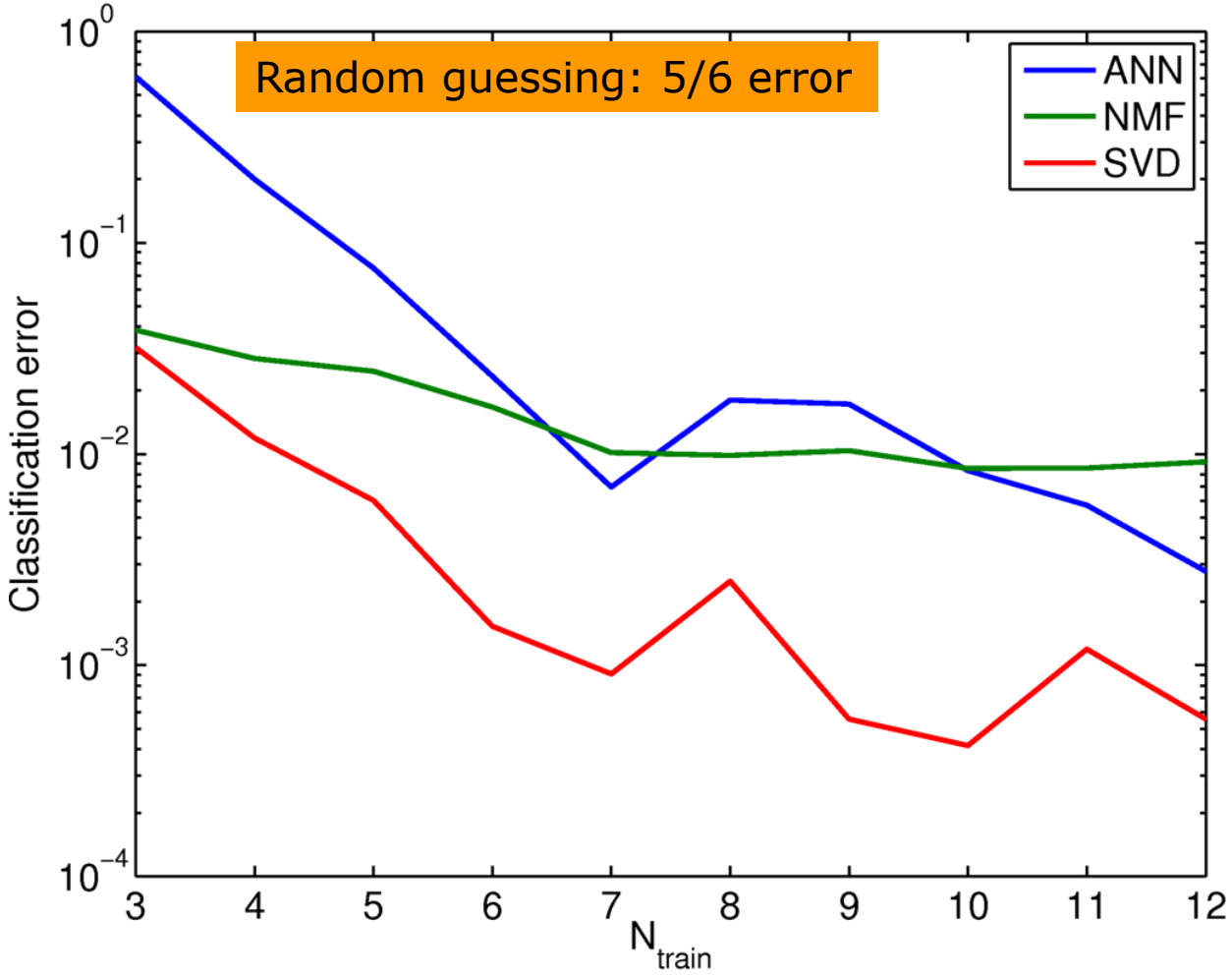
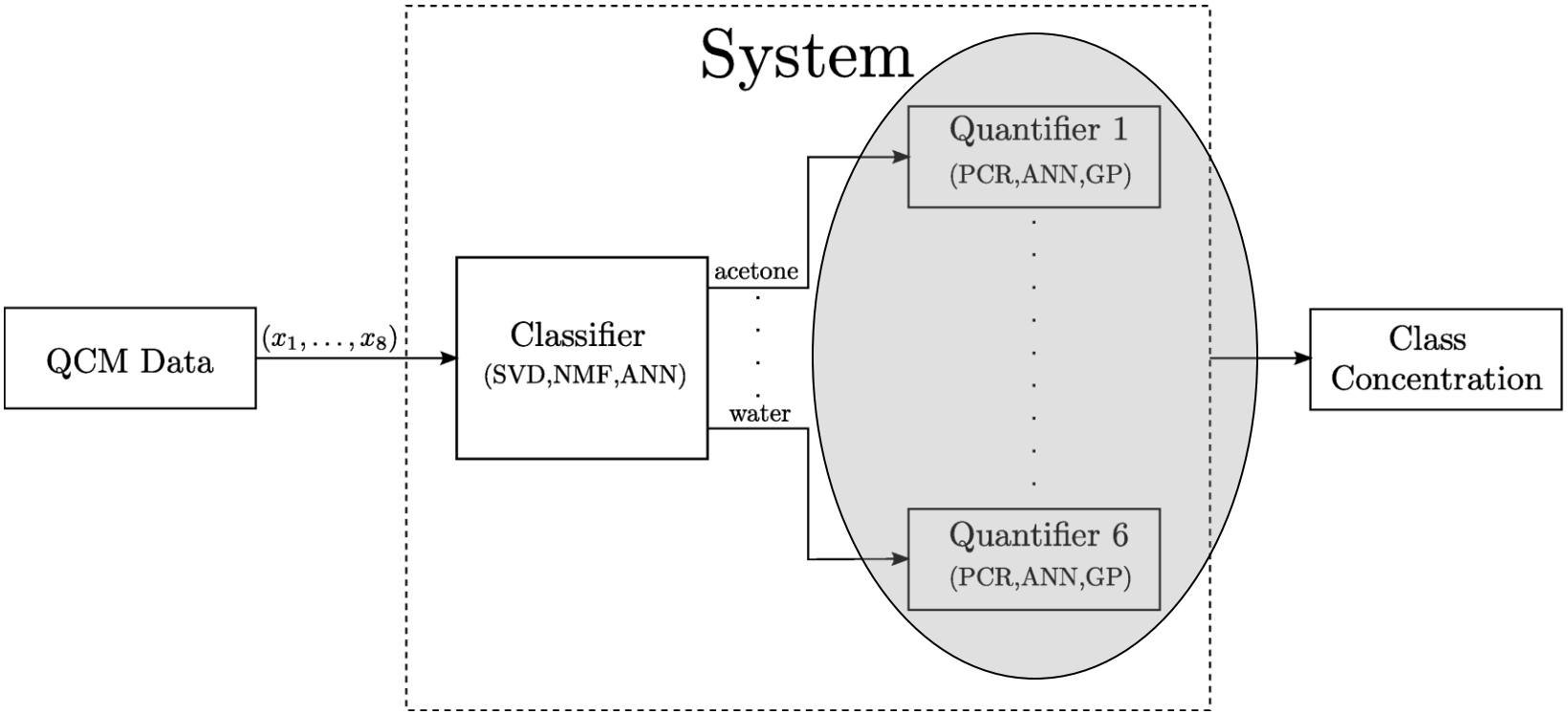


Classification results – average over 100 runs

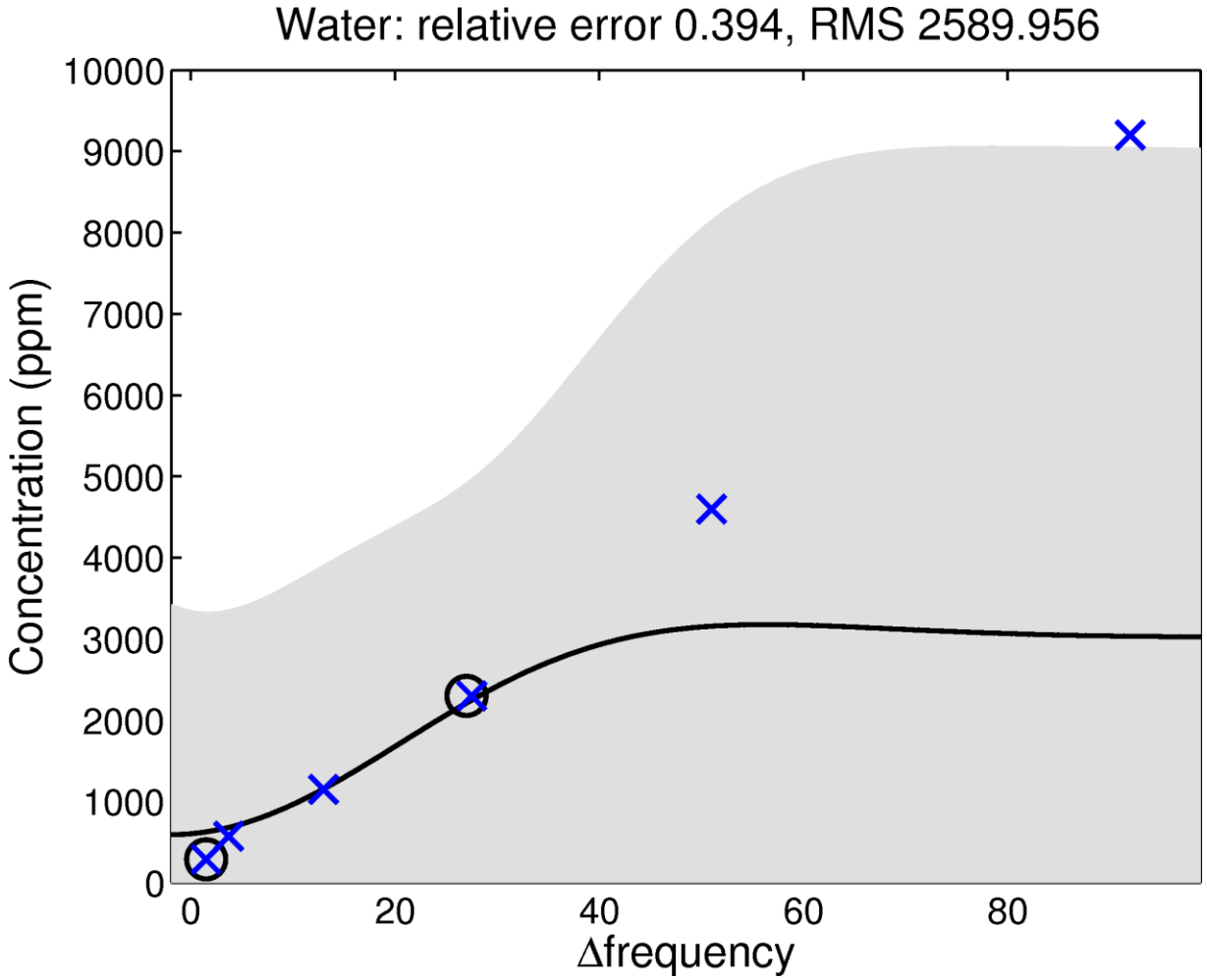
Data processing framework



Regression methods used

- Principal Component Regression (PCR)
  - A linear method that works well from few examples but are unable to model non-linear behavior
  - The model is simple to apply and requires little tuning
- Artificial Neural Networks (ANN)
  - A non-linear method that is an universal approximator.
  - Model requires careful regularization and optimization of hyper-parameters
- Gaussian Process Regression (GPR)
  - A non-linear method that is an universal approximator
  - Bayesian kernel regression method
  - Requires selection of covariance function

Gaussian Process demo on water using MAH



Performance evaluation of concentration level estimation

Estimated concentration

Relative Absolute Error

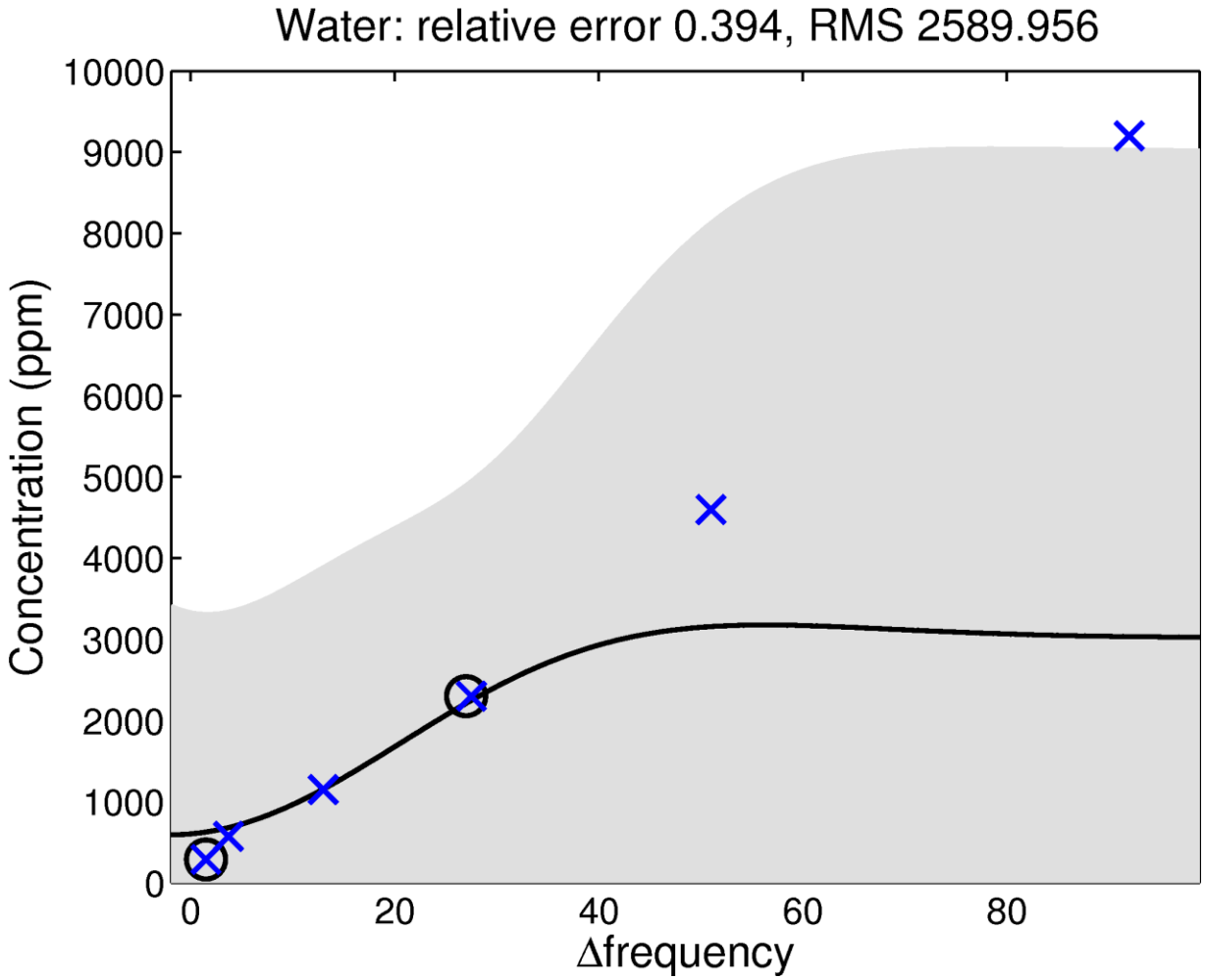
$$E(RAE) = \frac{1}{N}\sum_{n=1}^{N}\left|\frac{y_n - \hat{y}_n}{y_n}\right|$$

True concentration

Root Mean Square

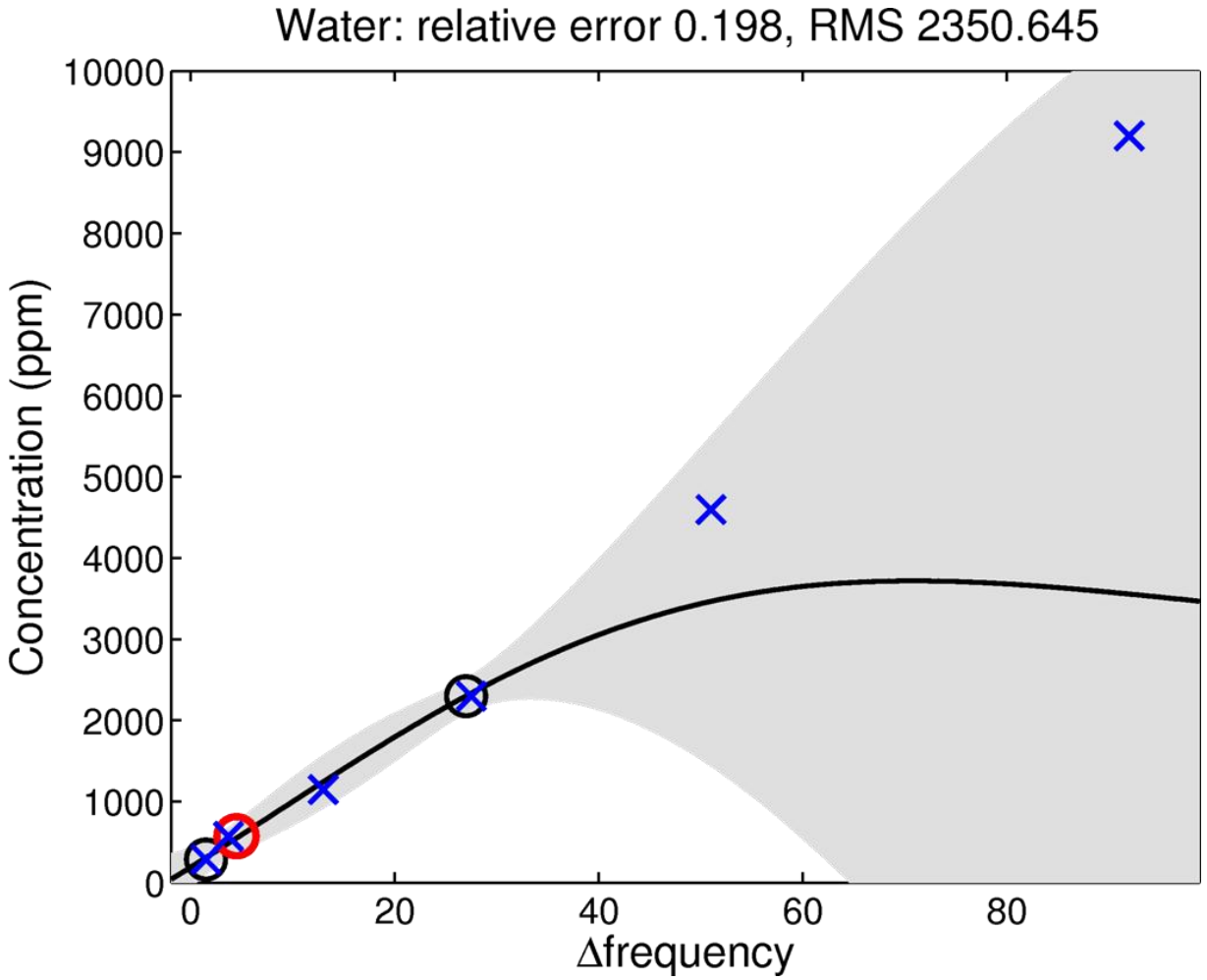
$$RMS = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2}$$

Gaussian Process demo on water using MAH



0.394

Gaussian Process demo on water using MAH



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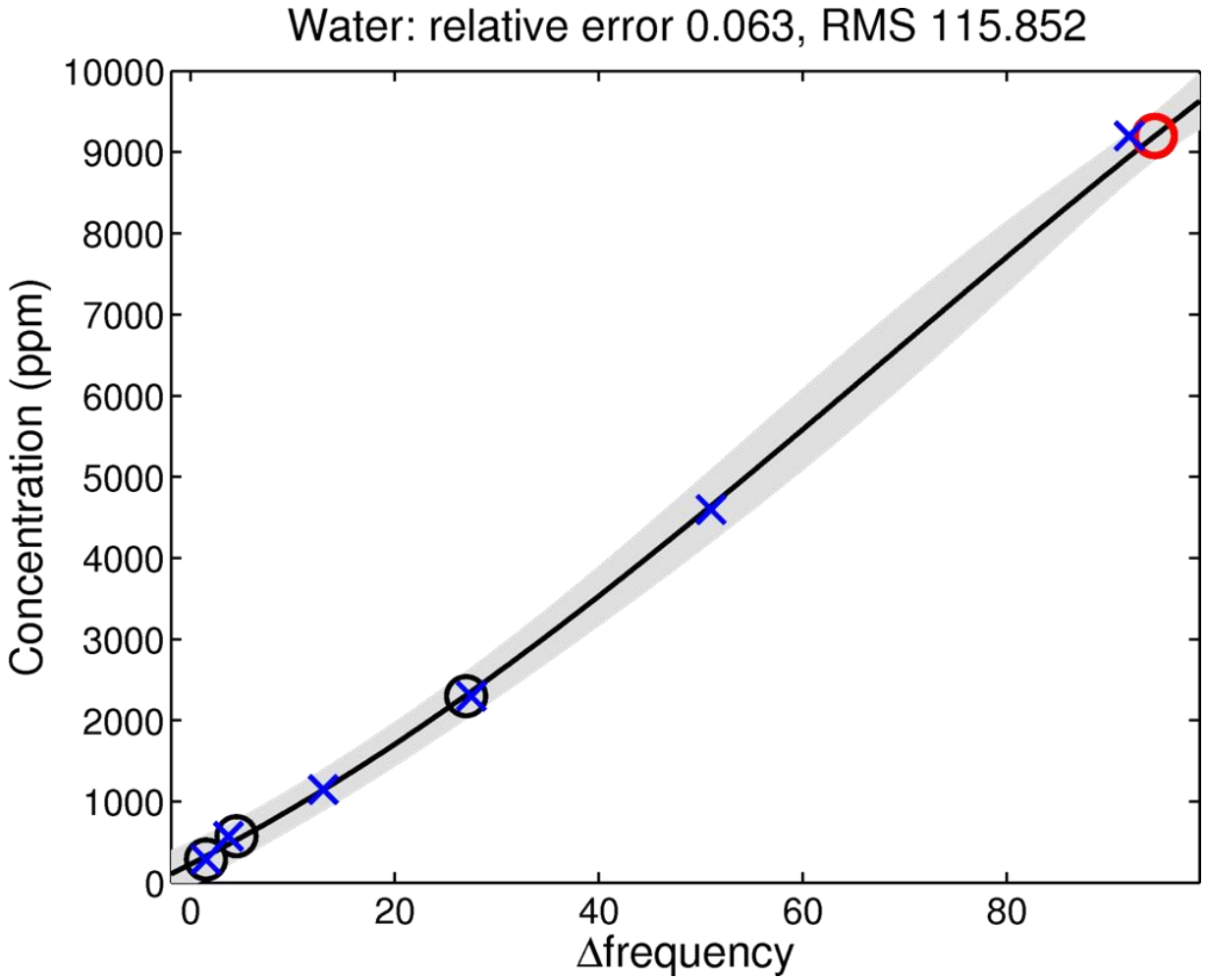
Gaussian Process demo on water using MAH



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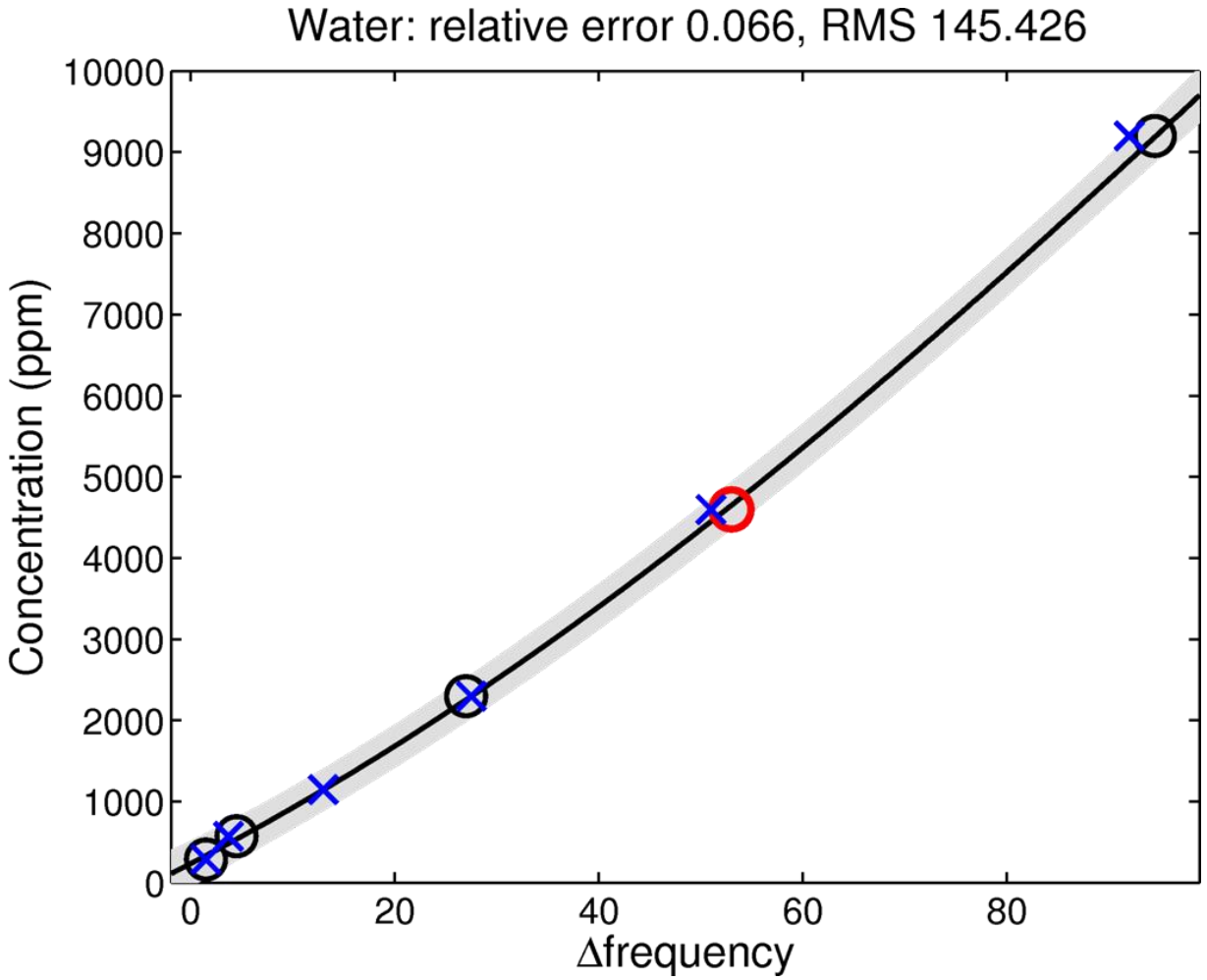
Gaussian Process demo on water using MAH



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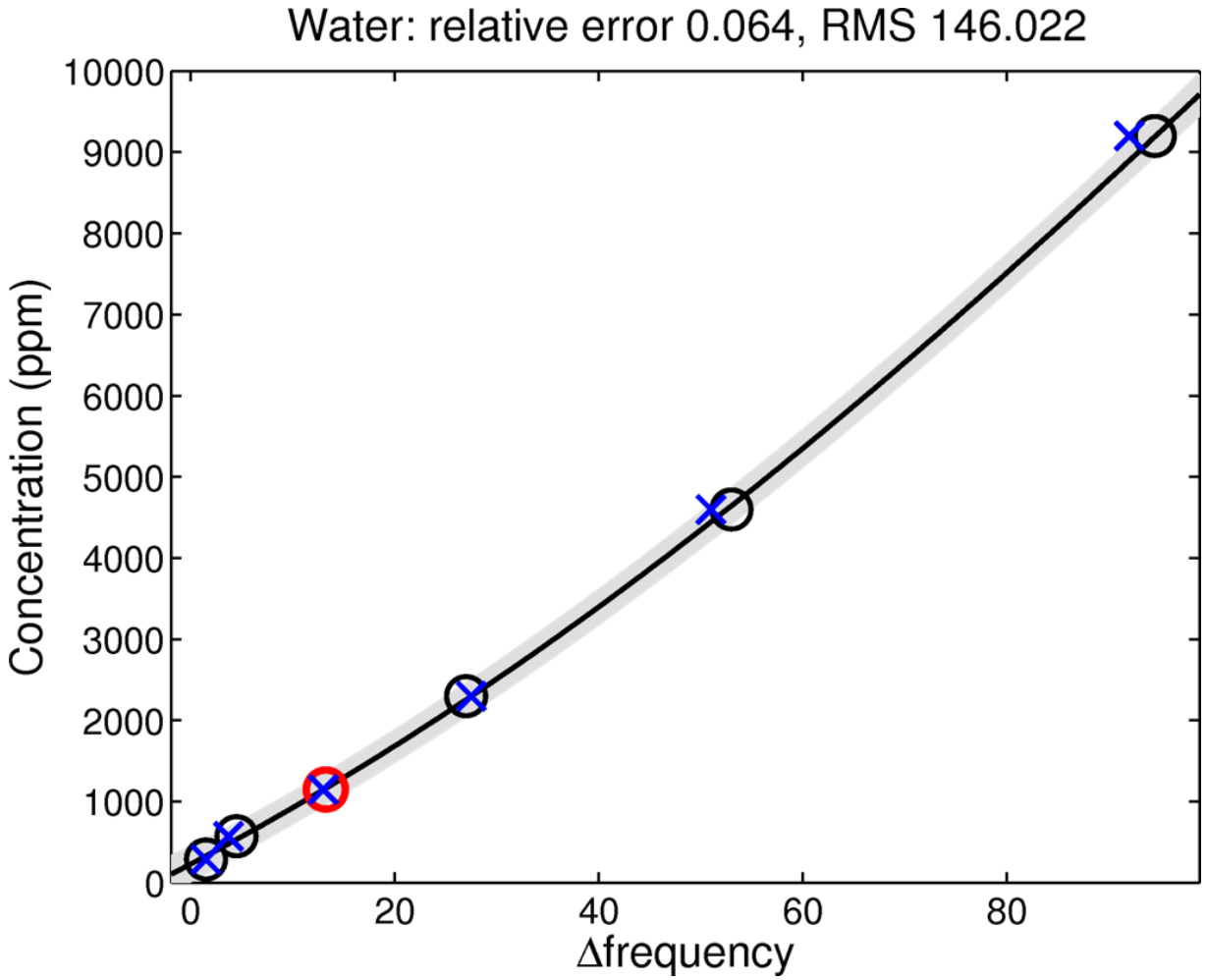
Gaussian Process demo on water using MAH



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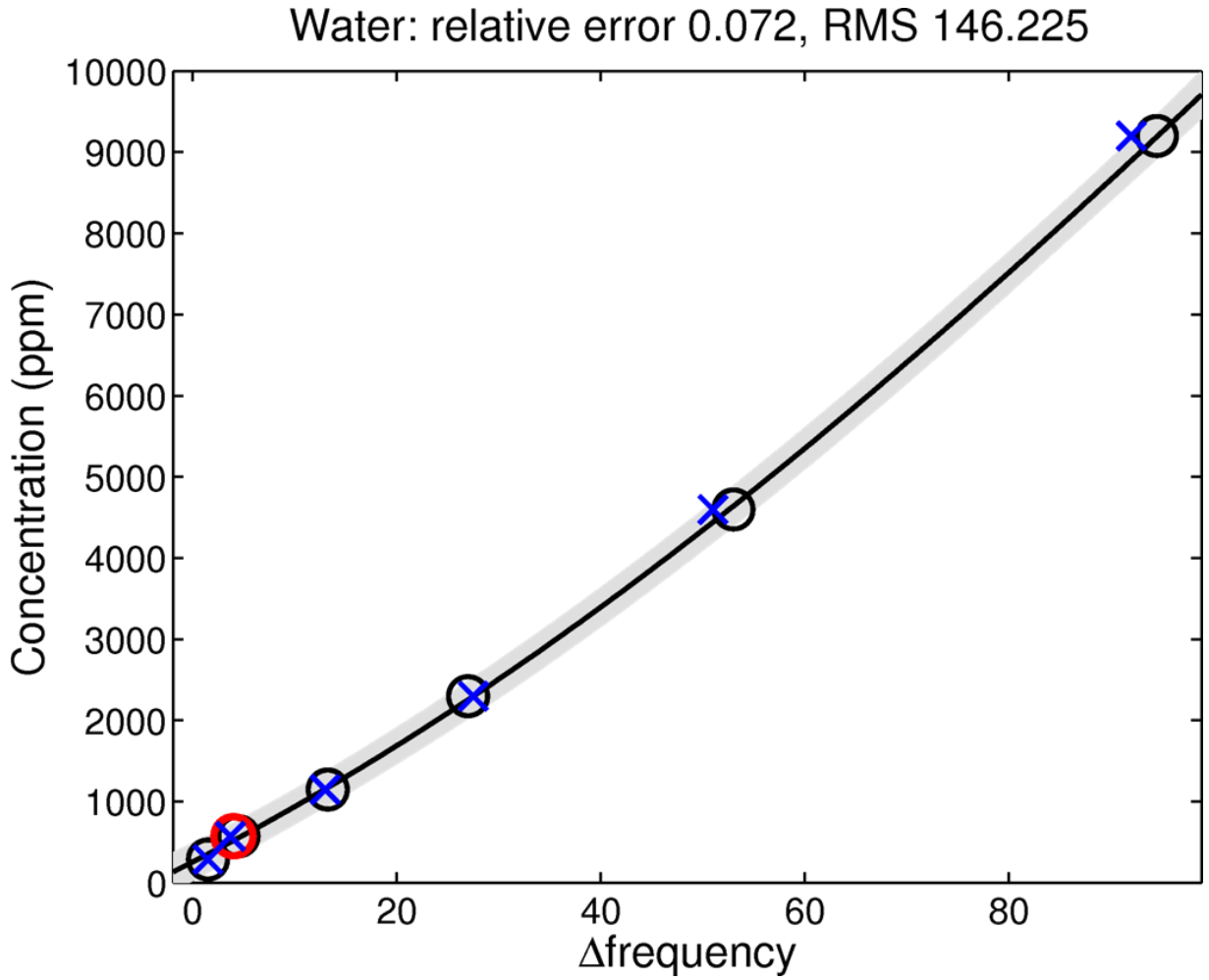
Gaussian Process demo on water using MAH



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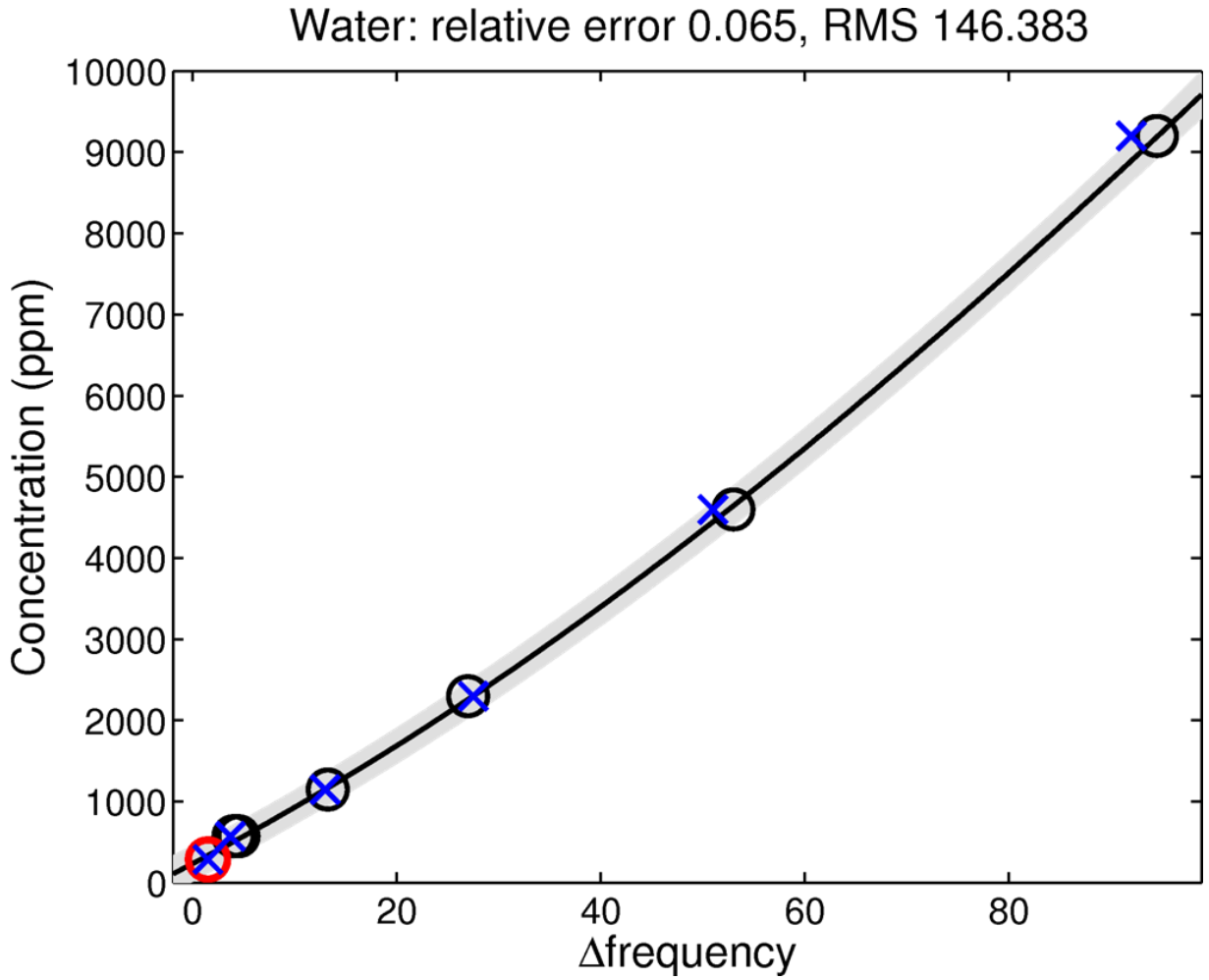
Gaussian Process demo on water using MAH



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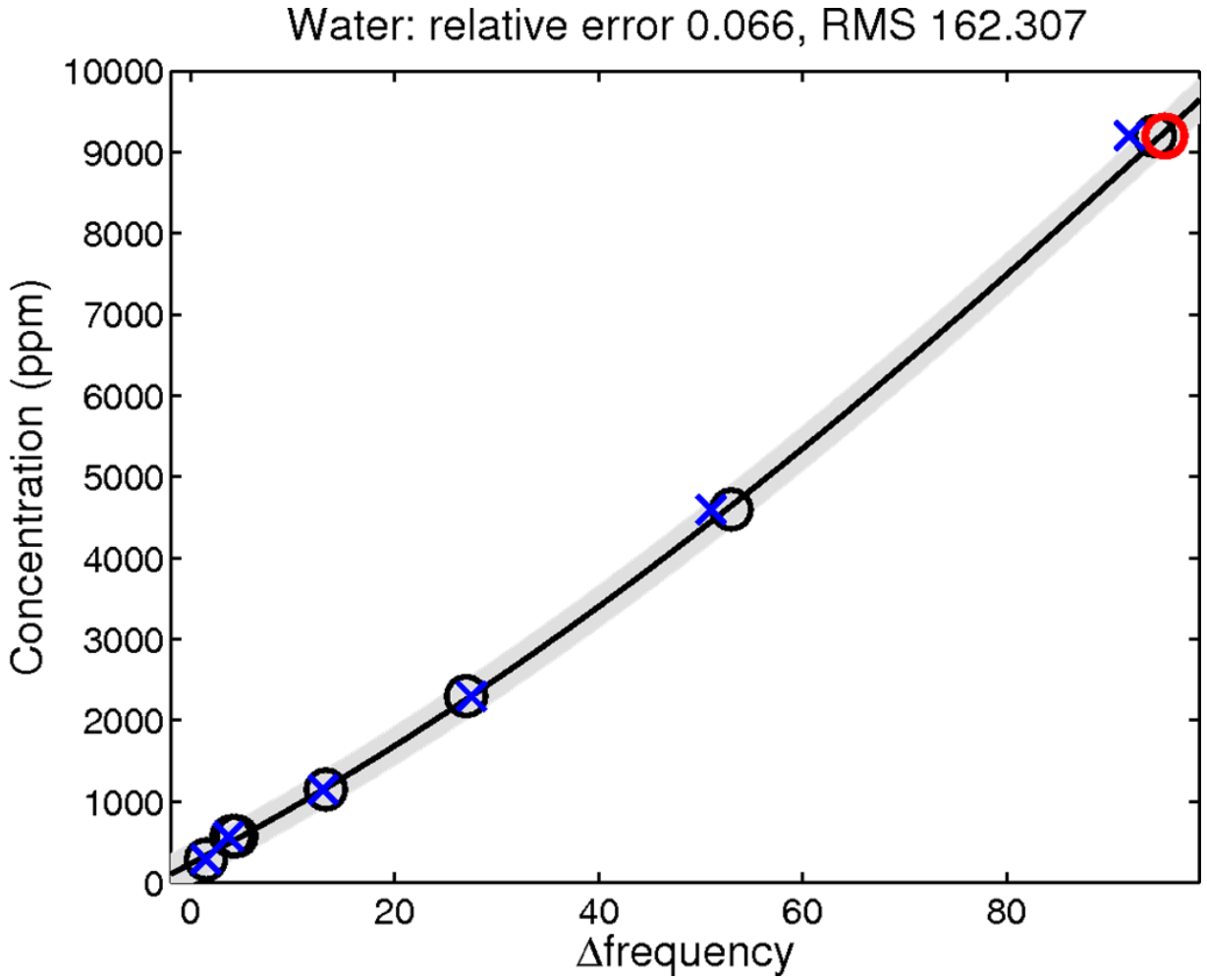
Gaussian Process demo on water using MAH



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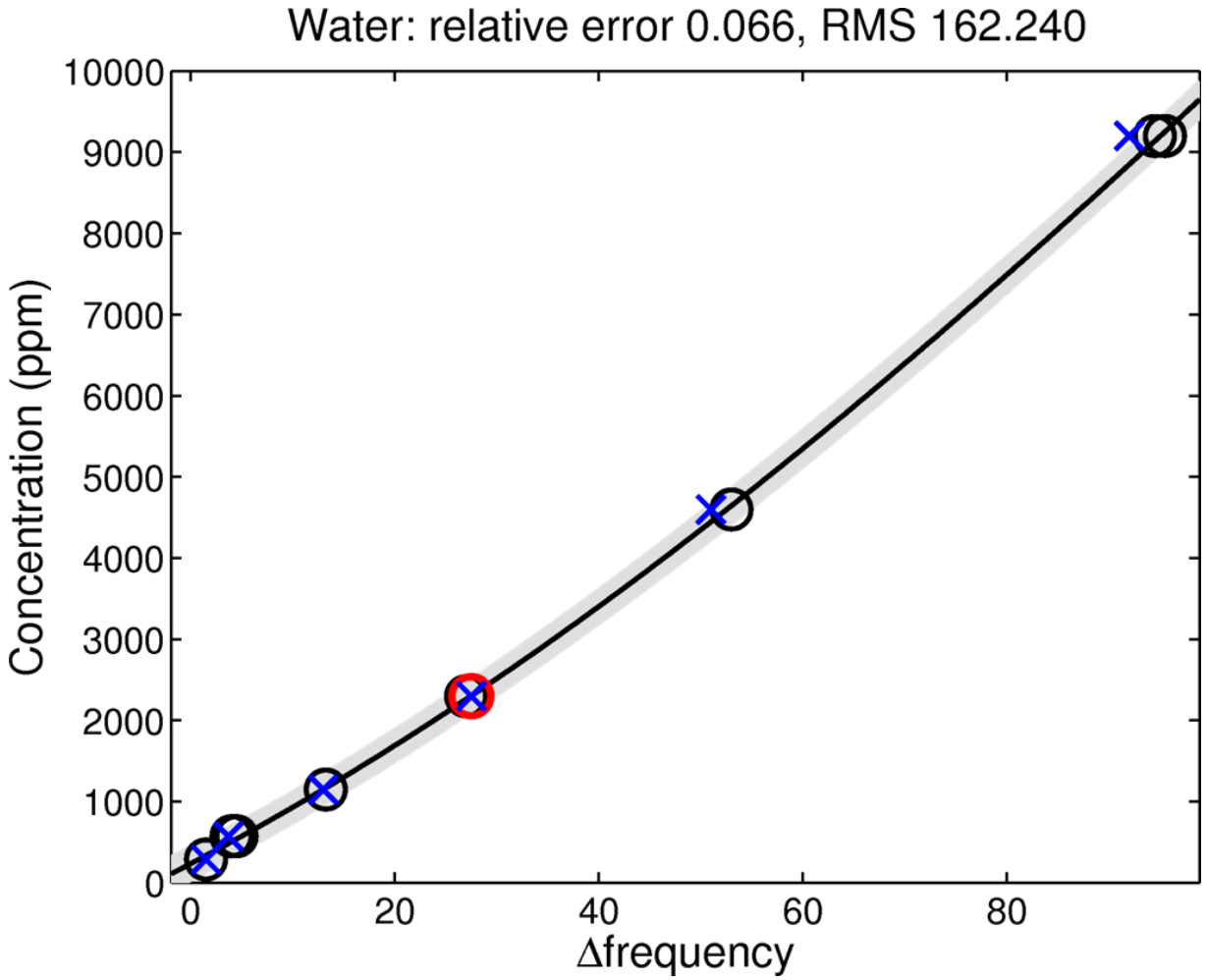

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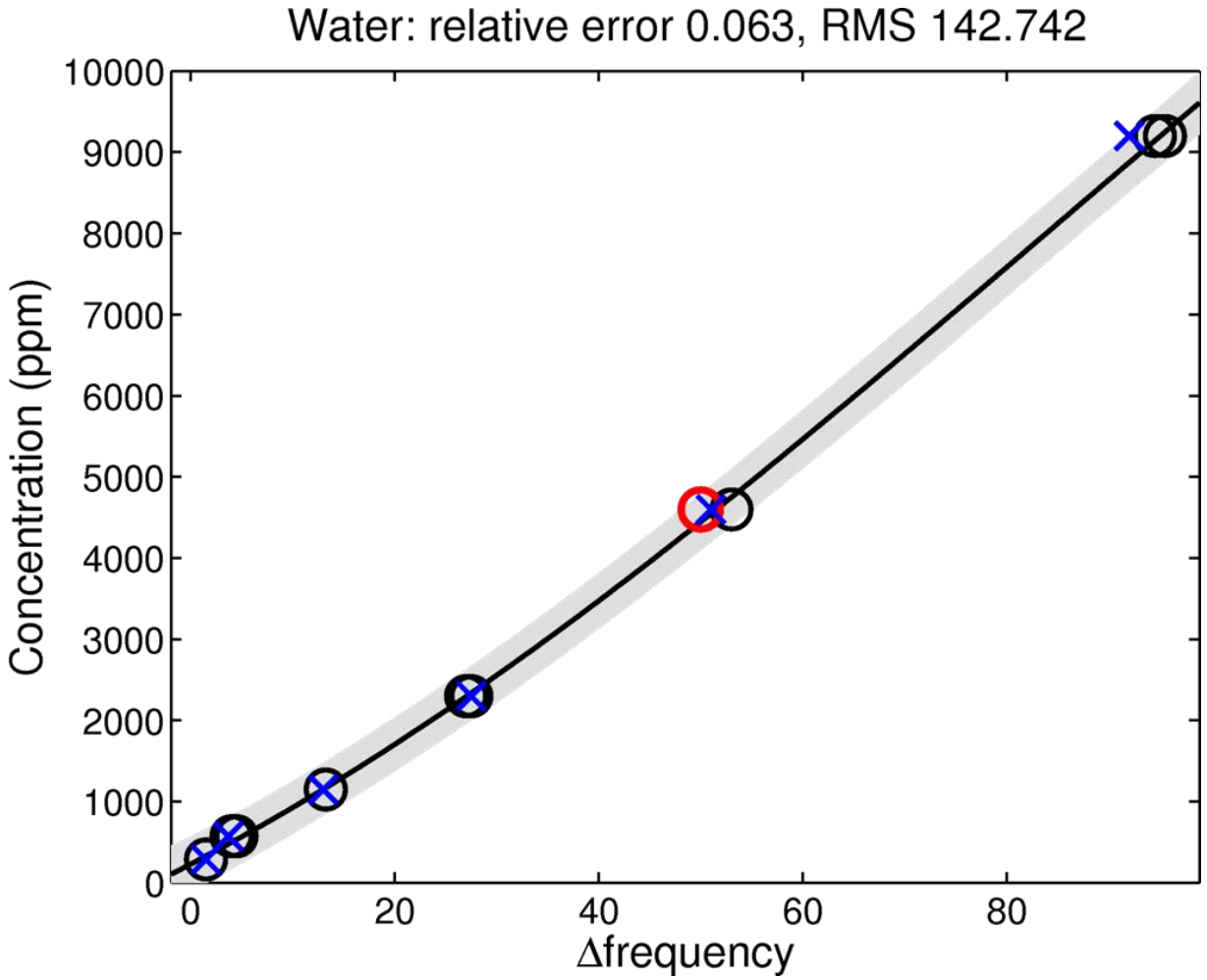

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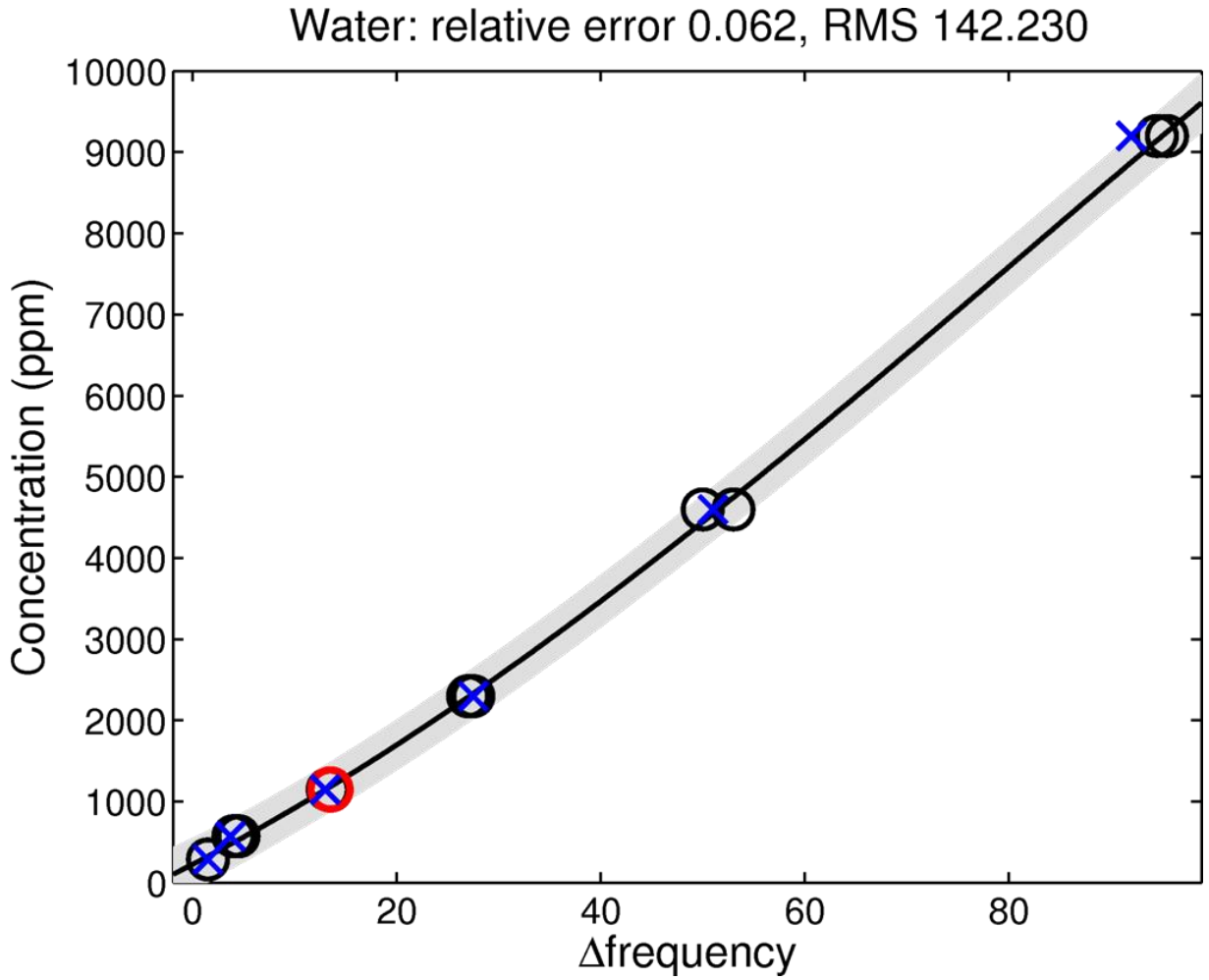

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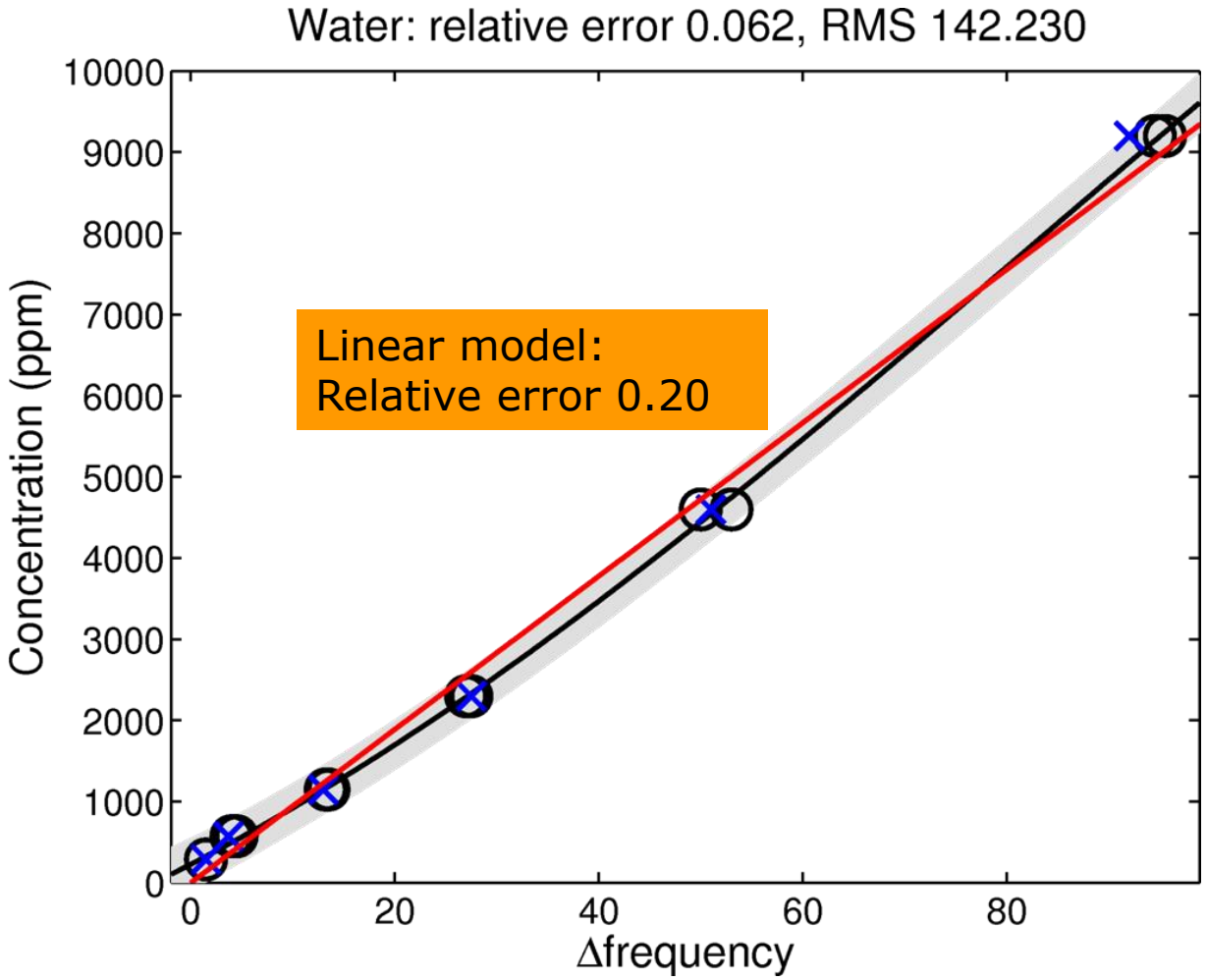

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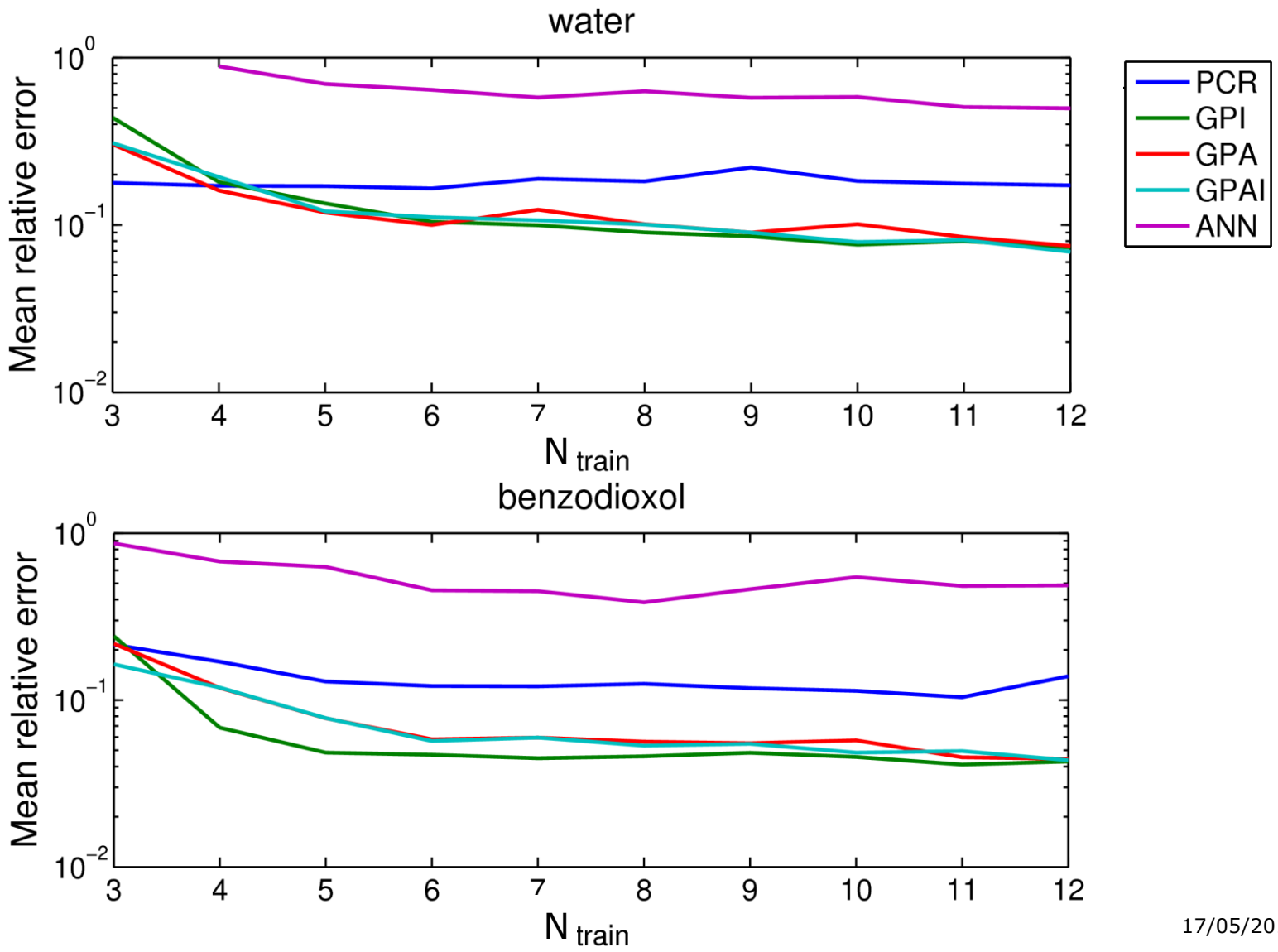
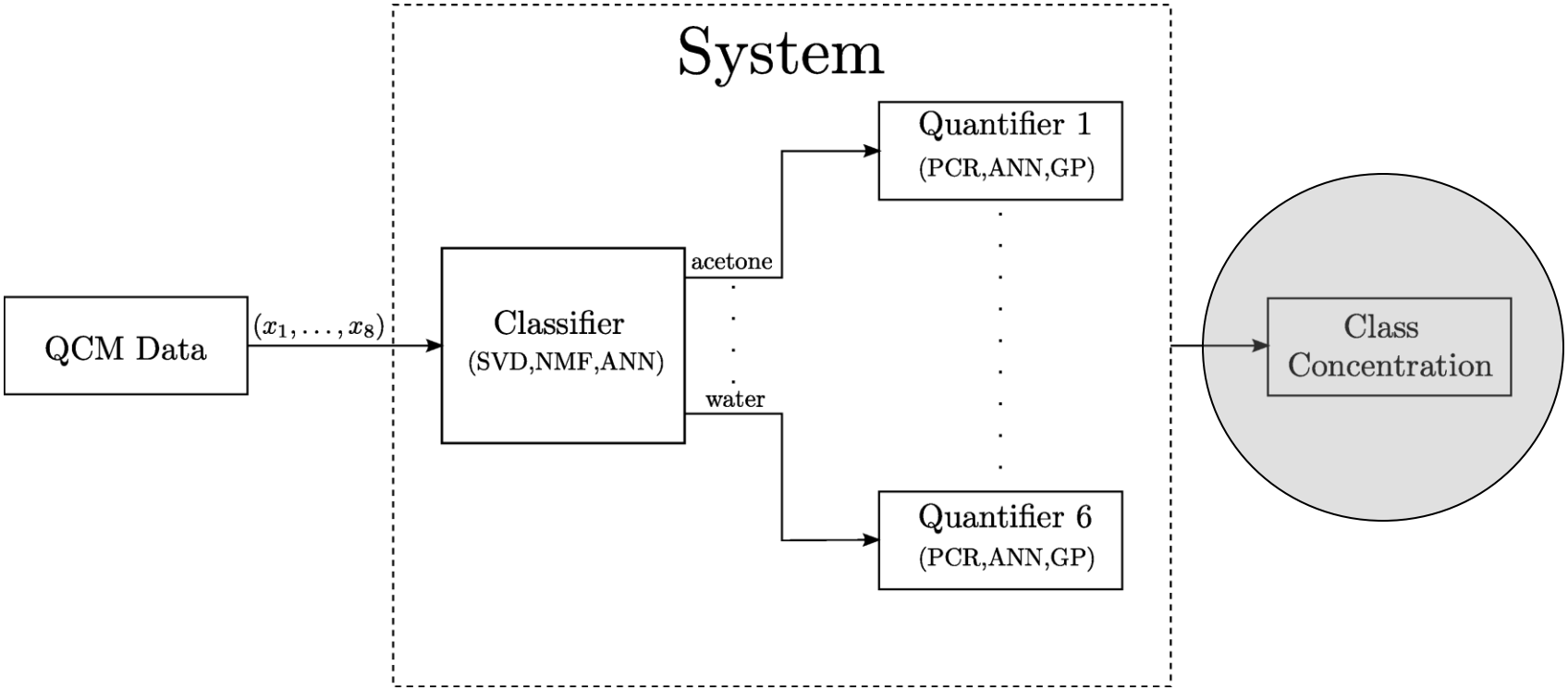
Concentration level estimation results

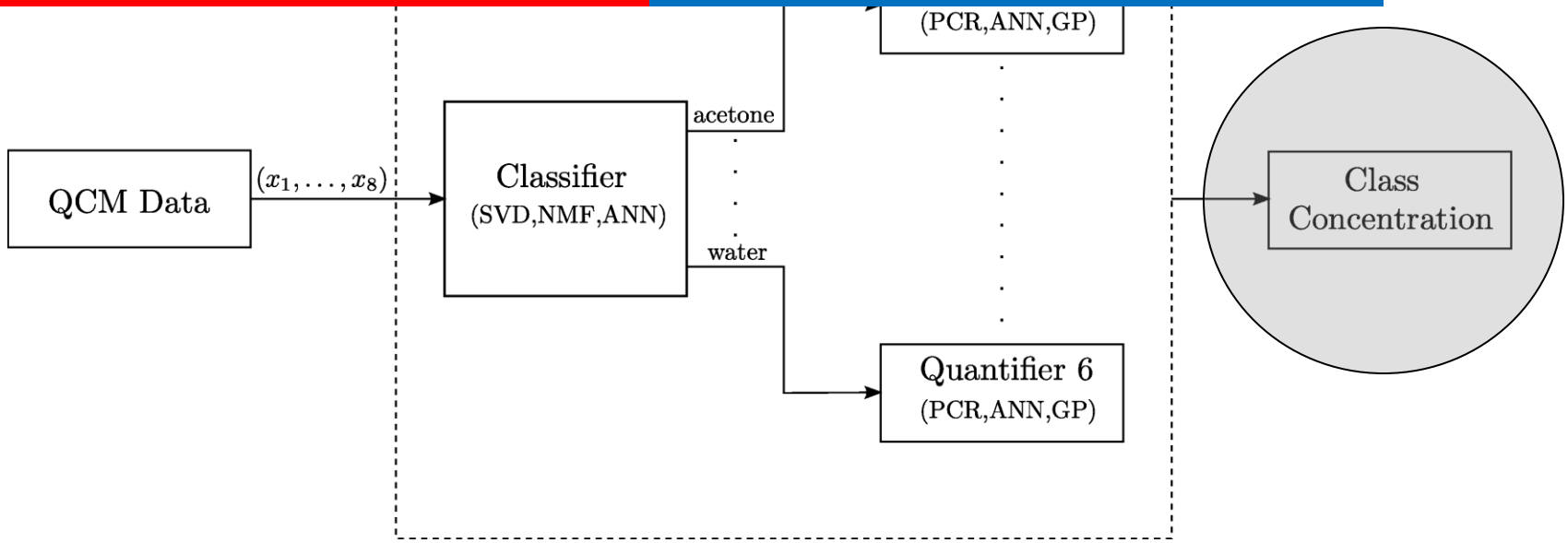


Data processing framework



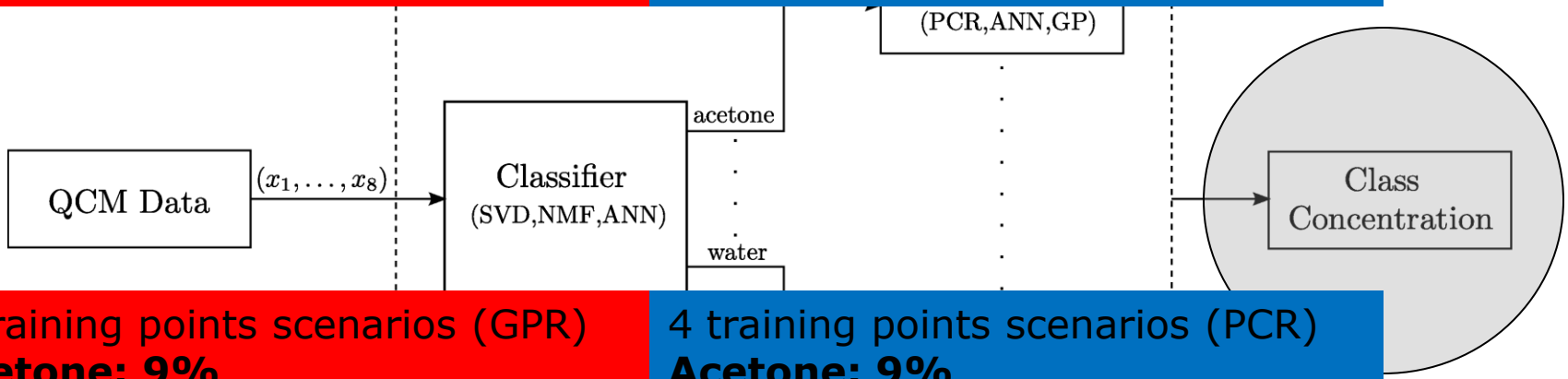
Concentration estimation
12 training points scenarios (GPR)
Acetone: 3%
Benzodioxol: 4%
Ethanol: 4%
Heptane: 13%
Pentanol: 4%
Water: 7%

Concentration estimation
12 training points scenarios (PCR)
Acetone: 7%
Benzodioxol: 14%
Ethanol: 4%
Heptane: 16%
Pentanol: 12%
Water: 17%



Concentration estimation
12 training points scenarios (GPR)
Acetone: 3%
Benzodioxol: 4%
Ethanol: 4%
Heptane: 13%
Pentanol: 4%
Water: 7%

Concentration estimation
12 training points scenarios (PCR)
Acetone: 7%
Benzodioxol: 14%
Ethanol: 4%
Heptane: 16%
Pentanol: 12%
Water: 17%



4 training points scenarios (GPR)
Acetone: 9%
Benzodioxol: 12%
Ethanol: 15%
Heptane: 23%
Pentanol: 19%
Water: 16%

4 training points scenarios (PCR)
Acetone: 9%
Benzodioxol: 17%
Ethanol: 9%
Heptane: 26%
Pentanol: 25%
Water: 17%

Conclusions

- The two-tiered data analysis framework works well
- The sensor is selective towards target analytes offering classification accuracy up to 99.9%. SVD and NMF offers 96% classification accuracy with 3 training points per analyte
- Classification accuracy implies that the choice of coatings represents a sufficient range of chemical interactions
- Gaussian Process regression works well for concentration level estimation – even when training points is limited

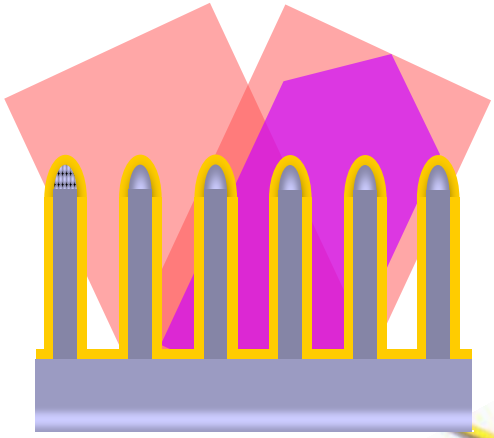
Future work

- Test the gas sensor on mixtures
- Improve concentration level estimation outside training interval by modifying the prior or the covariance function in GPR
- Apply polymer coatings to cantilever sensor

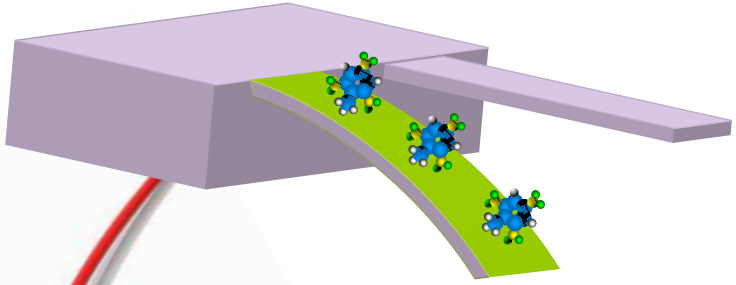
Xsense

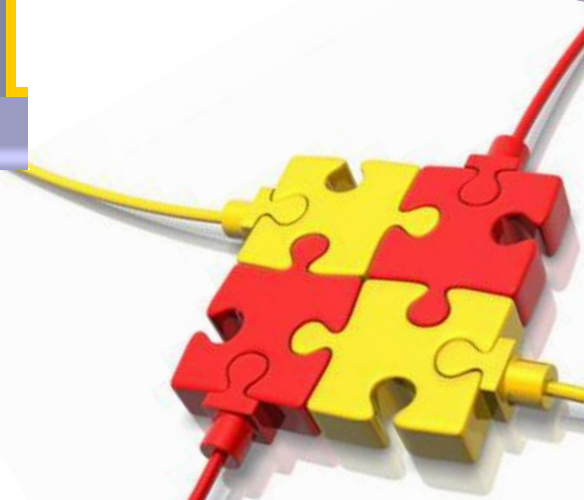
DTU

SERS

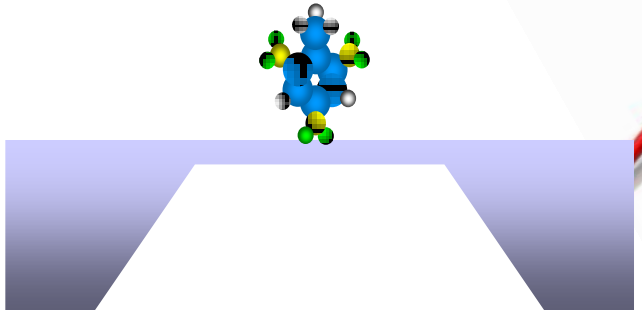


Cantilever

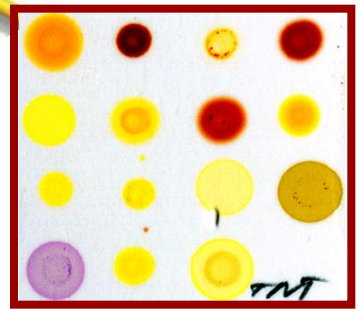




Calorimetric



Colorimetric



Monday 5 April

~~***Metal-coated silicon nanopillars with large Raman enhancement for explosive detection***~~ **[7673-02]**

Michael S. Schmidt

SESSION 1 Mon. 9:00 to 10:20 am

~~***Development of a colorimetric sensor array for detection of explosives in air***~~ **[7673-19]**

Natalie Kostesha

SESSION 4 Mon. 3:40 to 6:00 pm

Wednesday 7 April

Xsense: combining detection methods with nanotechnology for high-sensitivity handheld explosives detectors **[7664-51]**

Anja Boisen

SESSION 8 Wed. 2:40 to 6:00 pm

Thursday 8 April

POSTER SESSION Thurs. 6:00 to 7:30 pm

High-throughput readout system for cantilever-based sensing of explosive compounds **[7679-77]**

Filippo G. Bosco

Micro-calorimetric sensor for trace explosive particle detection **[7679-81]**

Jesper K. Olsen