Detection of chemical substances from colorimetric sensor data using probabilistic machine learning

CRIMTRACK

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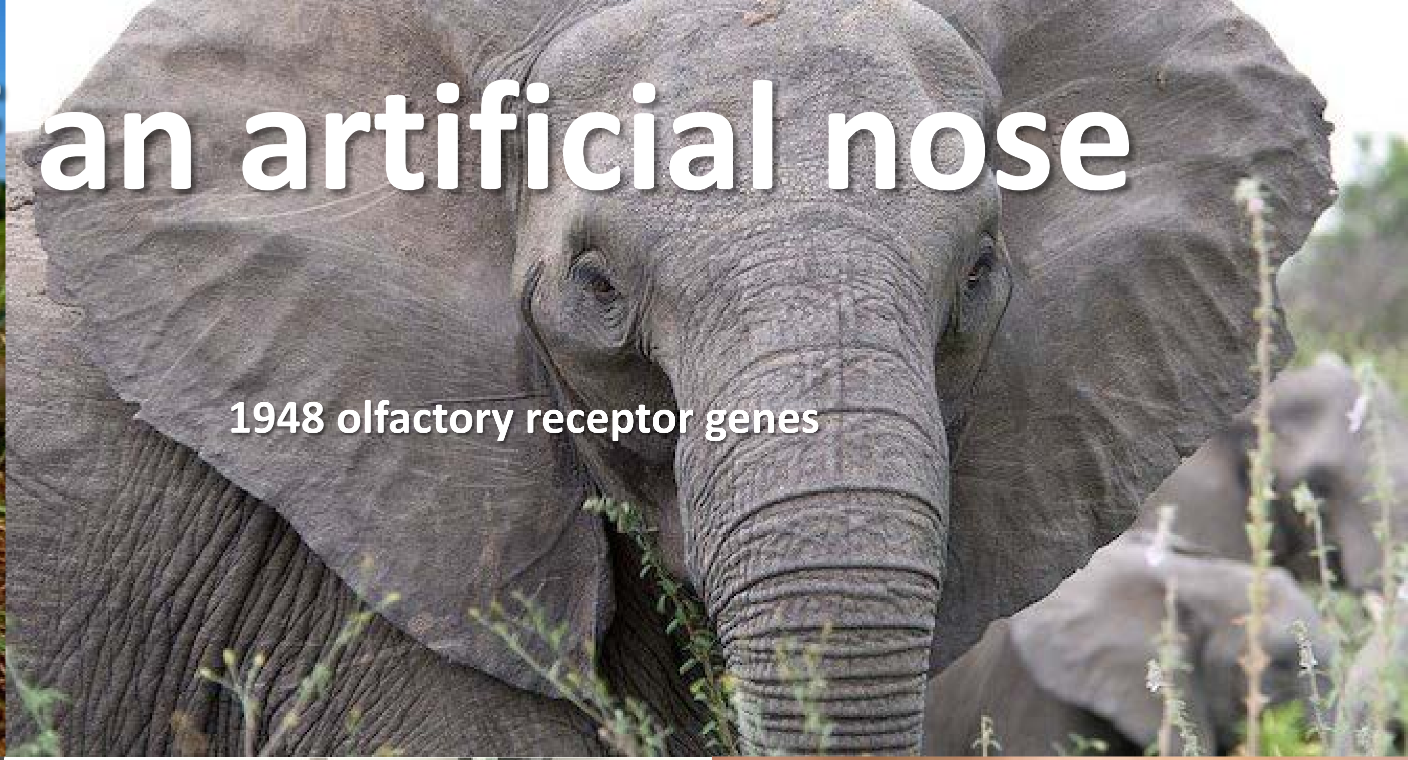
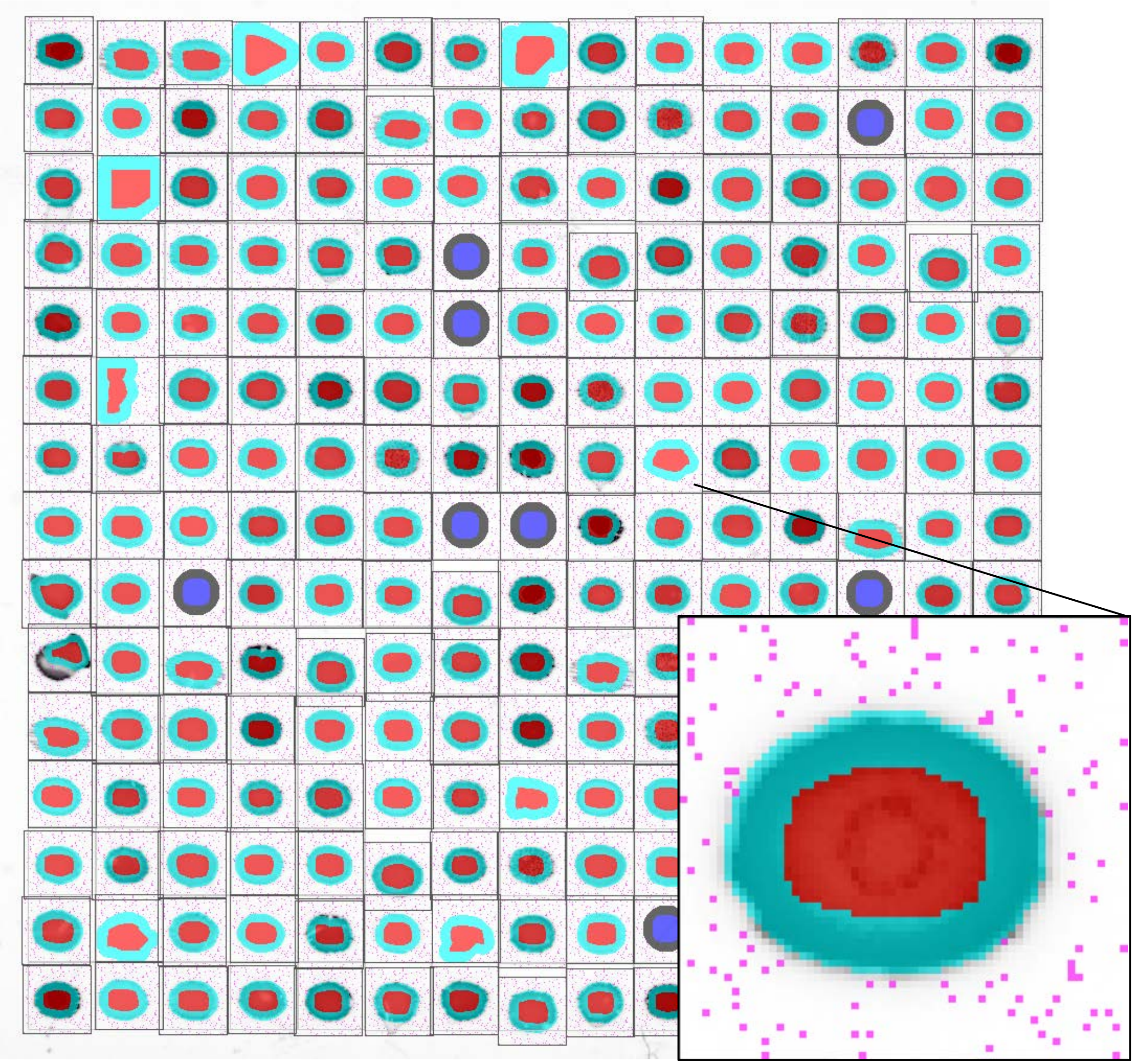
DREAM

The dream of an artificial nose



PRINCIPLE

Data conditioning and preprocessing – median RGB values for each dye

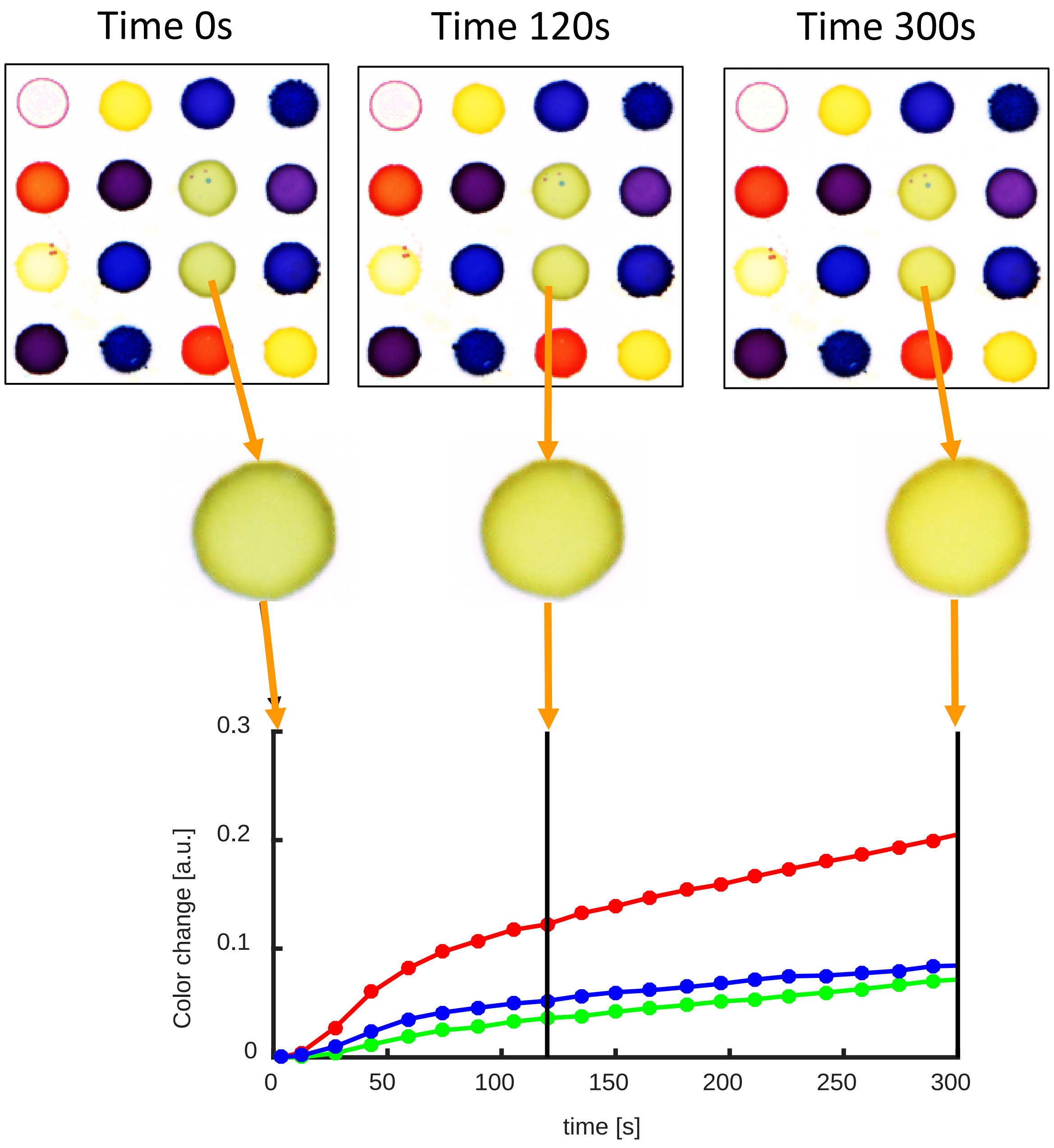


Extraction of color change

Dye spots are detected automatically.

RGB color changes are summarized as the relative color change to the pre-image at 0s.

The changes are small and requires sophisticated analysis.

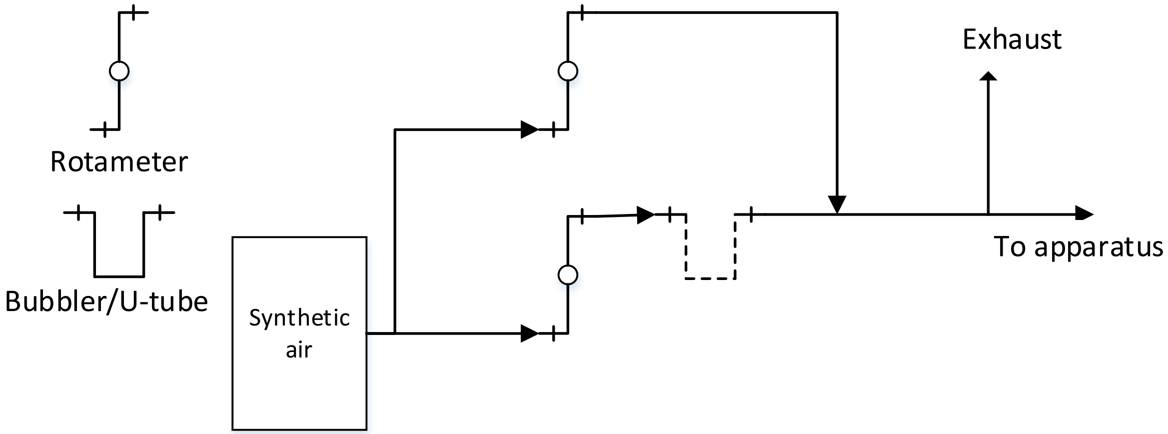


EXPERIMENTS

Experimental setup - two target analytes are investigated

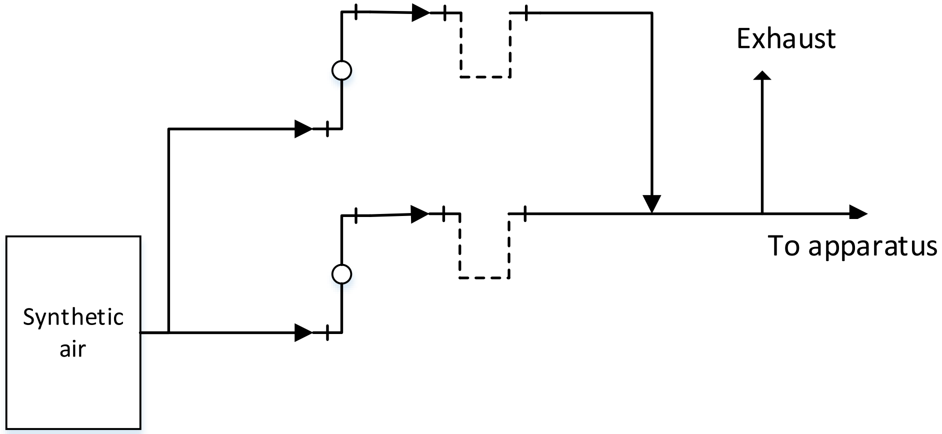
H_2O_2 - explosives precursor

– Generate different mixtures of synthetic air and analyte air samples
– Ratios between the target analyte and clean air: 0.1, 0.4, 0.7, and 1

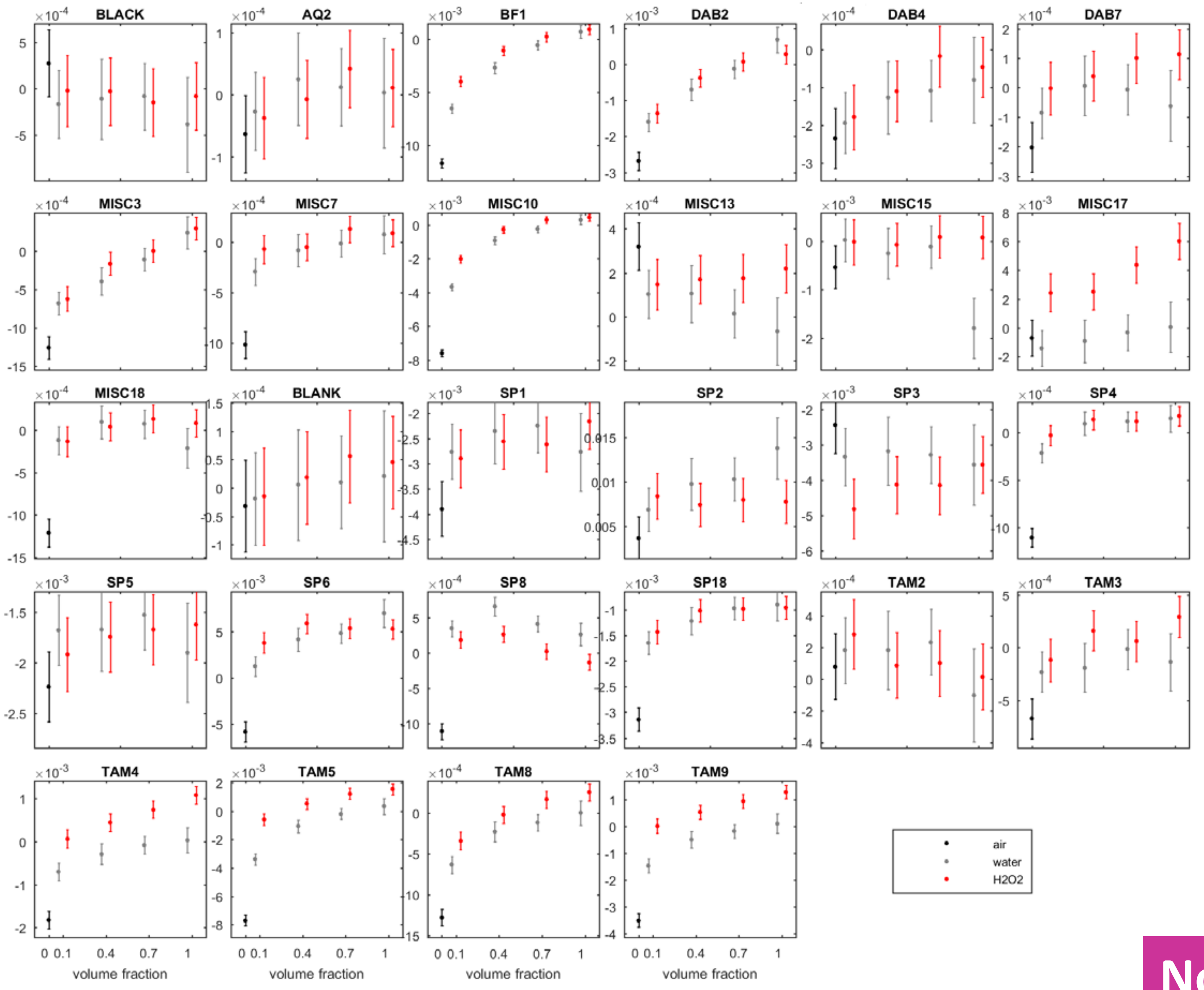


Phenylacetone (BMK) - illegal drug precursor

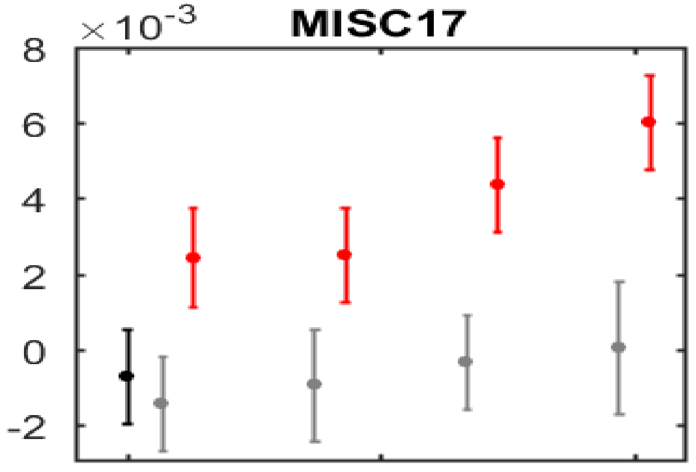
– Compare colorimetric response with naturally occurring confounders, i.e., acetone, diesel, gasoline, ethanol, water, and sea water.
– Clean samples of each substance obtained as well as mixtures of BMK with each confounder was measured.

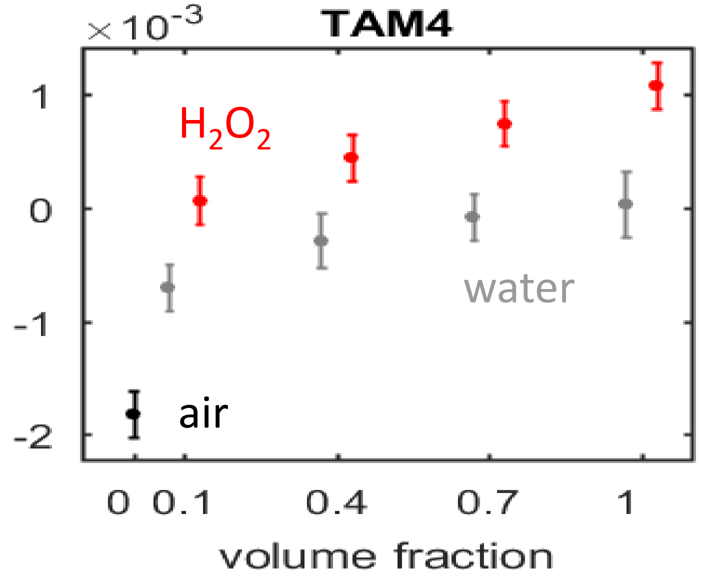


H_2O_2 dye color changes for dilution levels



Select good dyes

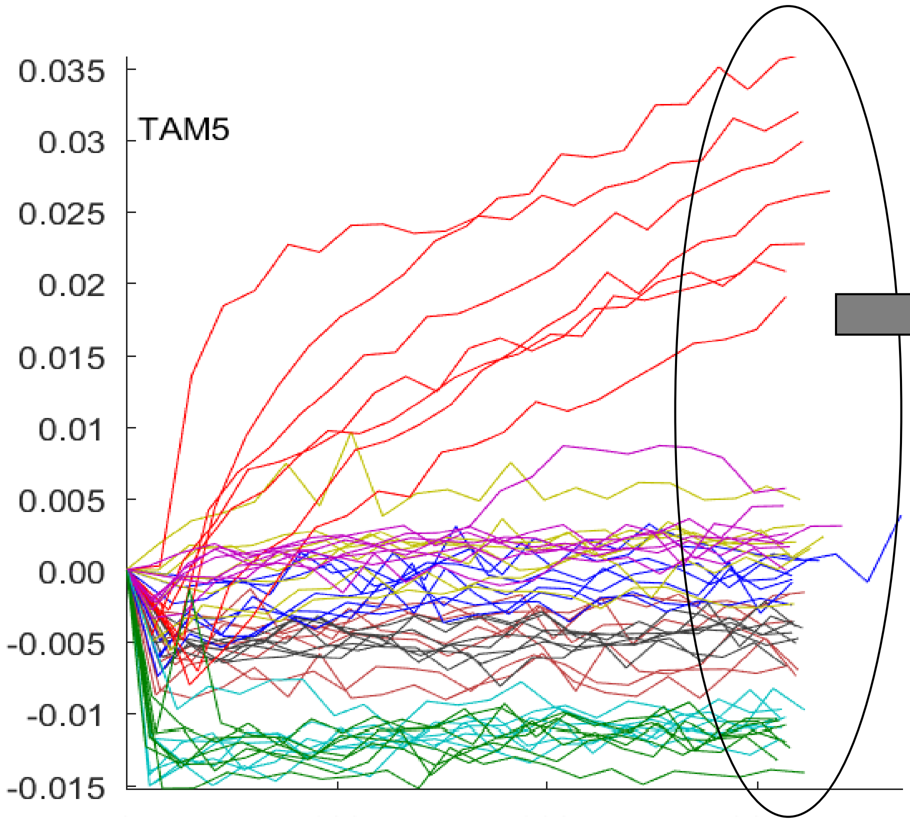




No single dye is sensitive enough!

DETECTION

Data processing pipeline

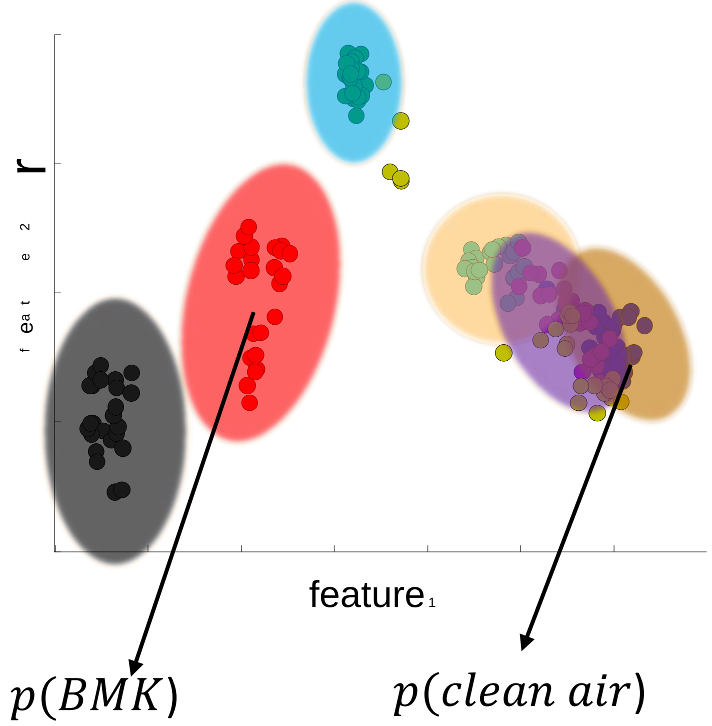


Extract color change (BMK experiments)

$$\begin{bmatrix} x_{BF1-r} \\ x_{BF1-g} \\ x_{BF1-1} \\ x_{DAB2-r} \\ x_{DAB2-g} \\ x_{DAB2-b} \\ \vdots \\ x_{TAM9-r} \\ x_{TAM9-g} \\ x_{TAM9-b} \end{bmatrix}$$

25 dyes x 3 color channels = 75 dim vector

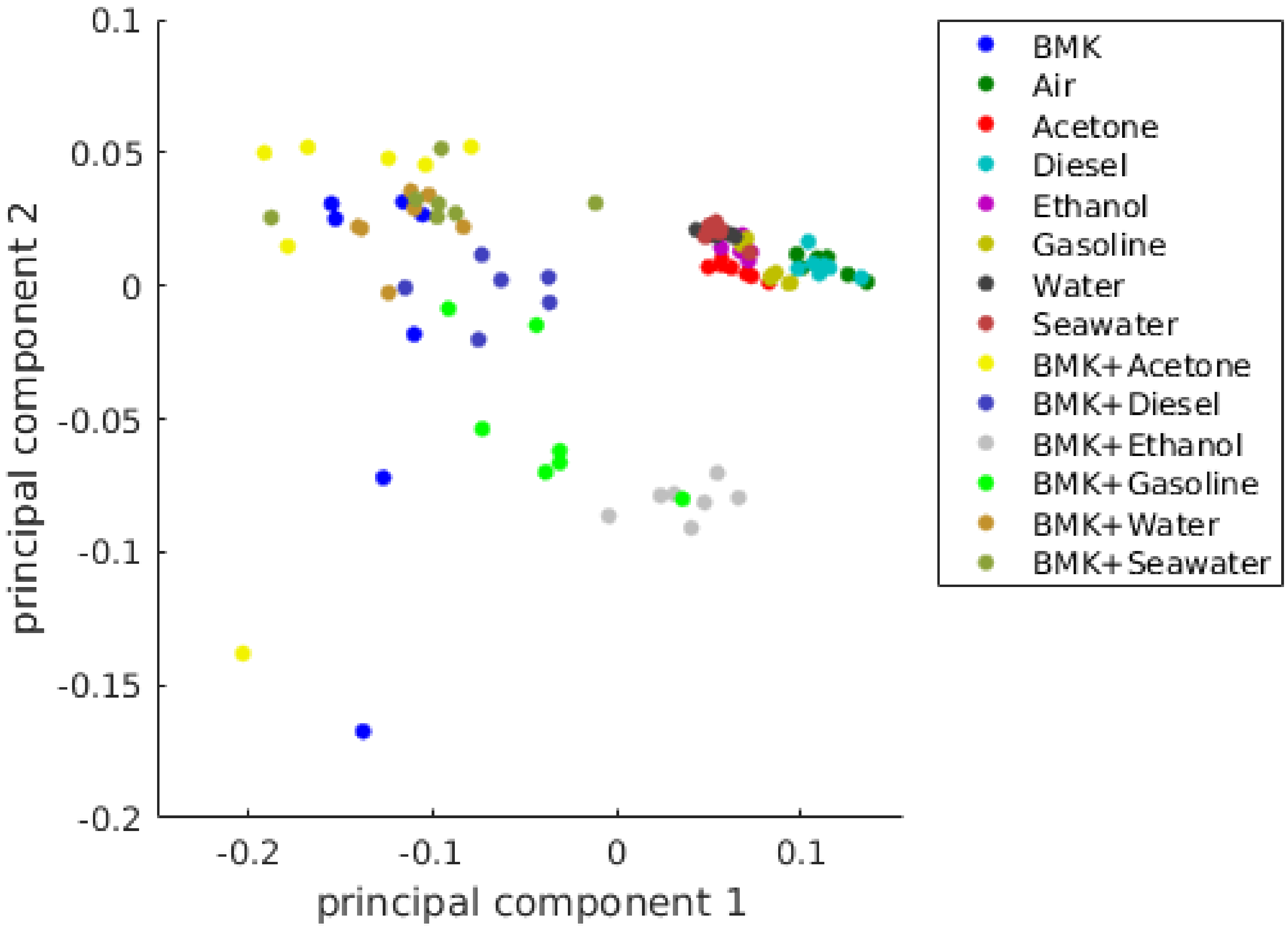
Adjust color change for nuisance factors (GLM-model)



Train classifier to find ”fingerprint” of target analyte

Includes choice of most useful dyes

BMK samples PCA visualization



Target
Confounders

Mixtures=target + confounders

Classification of BMK – 10 fold cross-validation

	KNN	logist. reg.	RF (no PCA)
BMK vs. confounders	97.3%	53.2%	100%
All BMK samples vs. confounders	100%	71%	100%
Train with clean BMK and confounders/ test on BMK mixtures	53%		86%

Classification of H_20_2 – 10 fold cross-validation

	KNN	logist. reg.	RF (no PCA)
H_2O_2	94.3%	75%	95%

KNN

		H_2O_2	confounder
True class	H_2O_2	36	4
	confounder	1	46

log.reg.

		H_2O_2	confounder
True class	H_2O_2	39	1
	confounder	20	27

RF

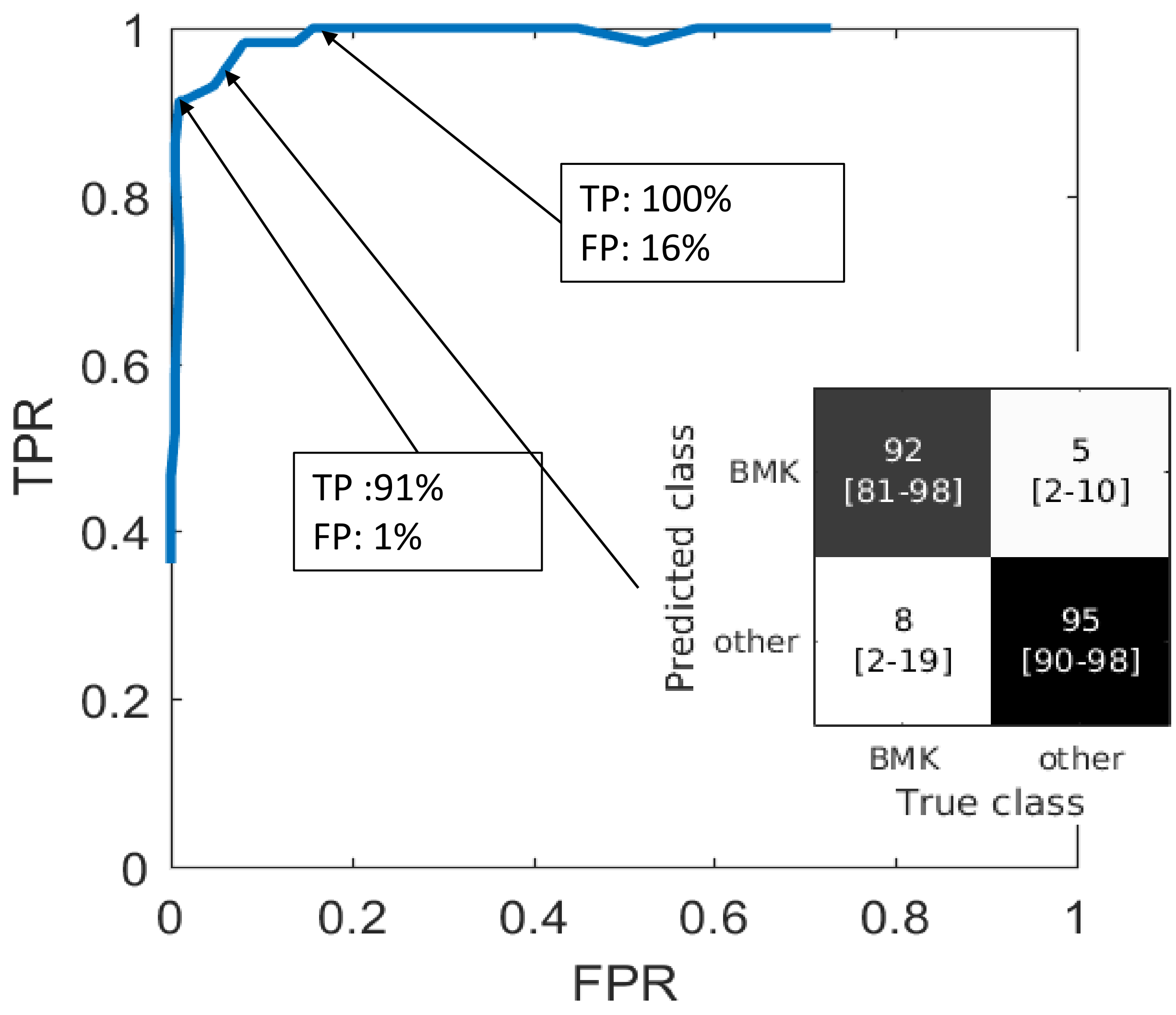
		H_2O_2	confounder
True class	H_2O_2	38	2
	confounder	2	45

USE-CASE RESULTS

Detecting 100 µl BMK in a box

- BMK end-user campaign focused on discriminating BMK from ambient air, water vapor, and acetone.

- Training on 176 samples. Expected performance evaluated on hold-out test set.



Detecting 50 mg HMTD in a box

- HMTD end-user campaign focused on discriminating HMTD from ambient air, water vapor, and H_2O_2.

- Training on 350 samples. Expected performance evaluated using hold-out test set.