DTU

Improved detection of chemical substances from colorimetric sensor data using probabilistic machine learning

CRIMTRACK

Lasse L. Mølgaard, Ole T. Buus, **Jan Larsen**, Hamid Babamoradi, Ida L. Thygesen, Milan Laustsen, Jens Kristian Munk, Eleftheria Dossi, Caroline O'Keeffe, Lina Lässig, Sol Tatlow, Lars Sandström, and Mogens H. Jakobsen

Section for Cognitive Systems, DTU Compute, Richard Petersens Plads, Building 324, 2800 Kongens Lyngby, Denmark

Partners

P1: DTU (University) DK	Danmarks Tekniske Universitet DTU	P2: CRA (University) UK	Cranfield UNIVERSITY
P3: SEC (SME) DE	SECURETEC DETEKTIONS-SYSTEME AG	P4: PDE (SME) DE	prodesign electronic gmbh
P5: GIAB (SME) SE	gammadata INSTRUMENT	P6: DCL (LEA) NL	Dutch Customs Laboratory
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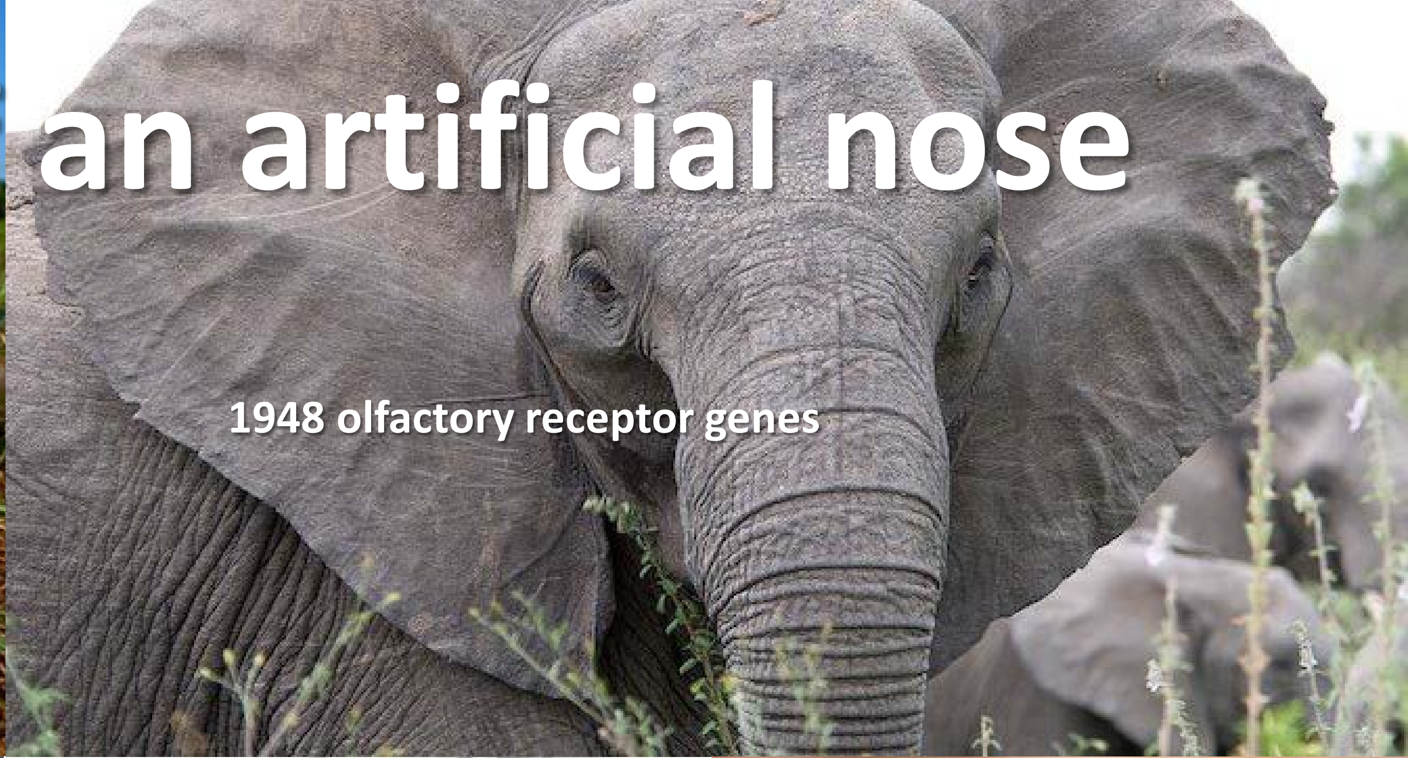
The dream of an artificial nose



The CRIM-TRACK Sniffer System

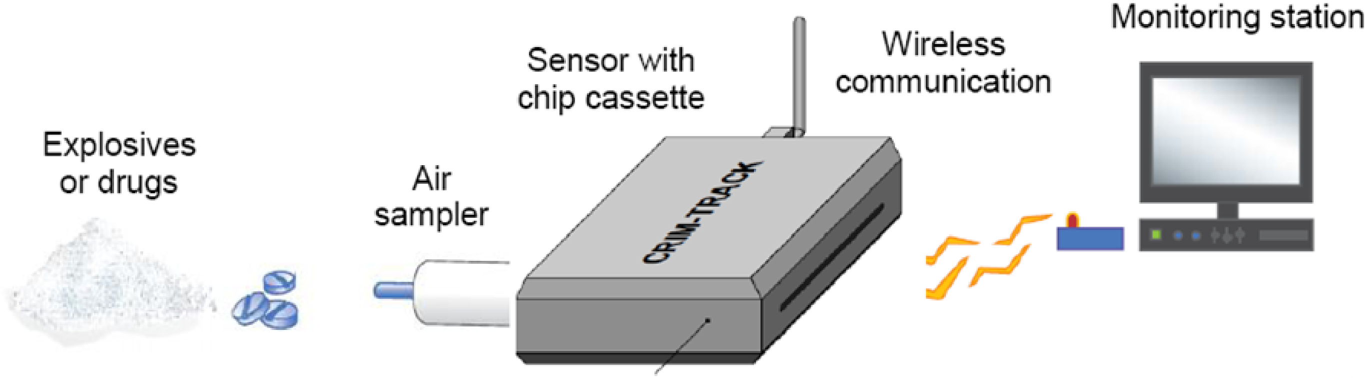


Figure 3: Outline of the Sniffer components

Monitoring station:

- Servicing multiple CRIM-TRACK sensors
- User independent interpretation of results based on machine learning

Air sampler:

- Low volume (portable)
- High volume (container traffic)

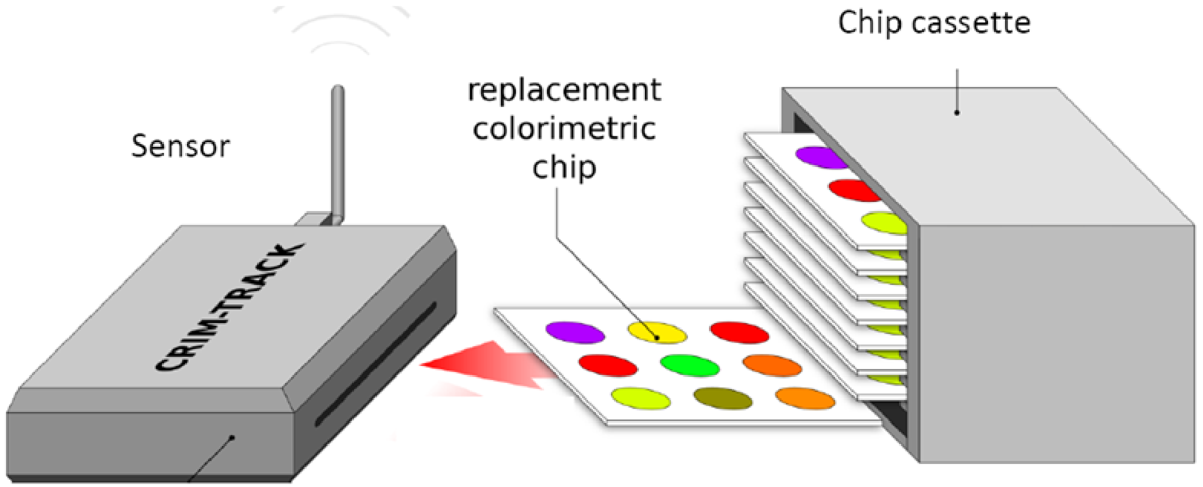
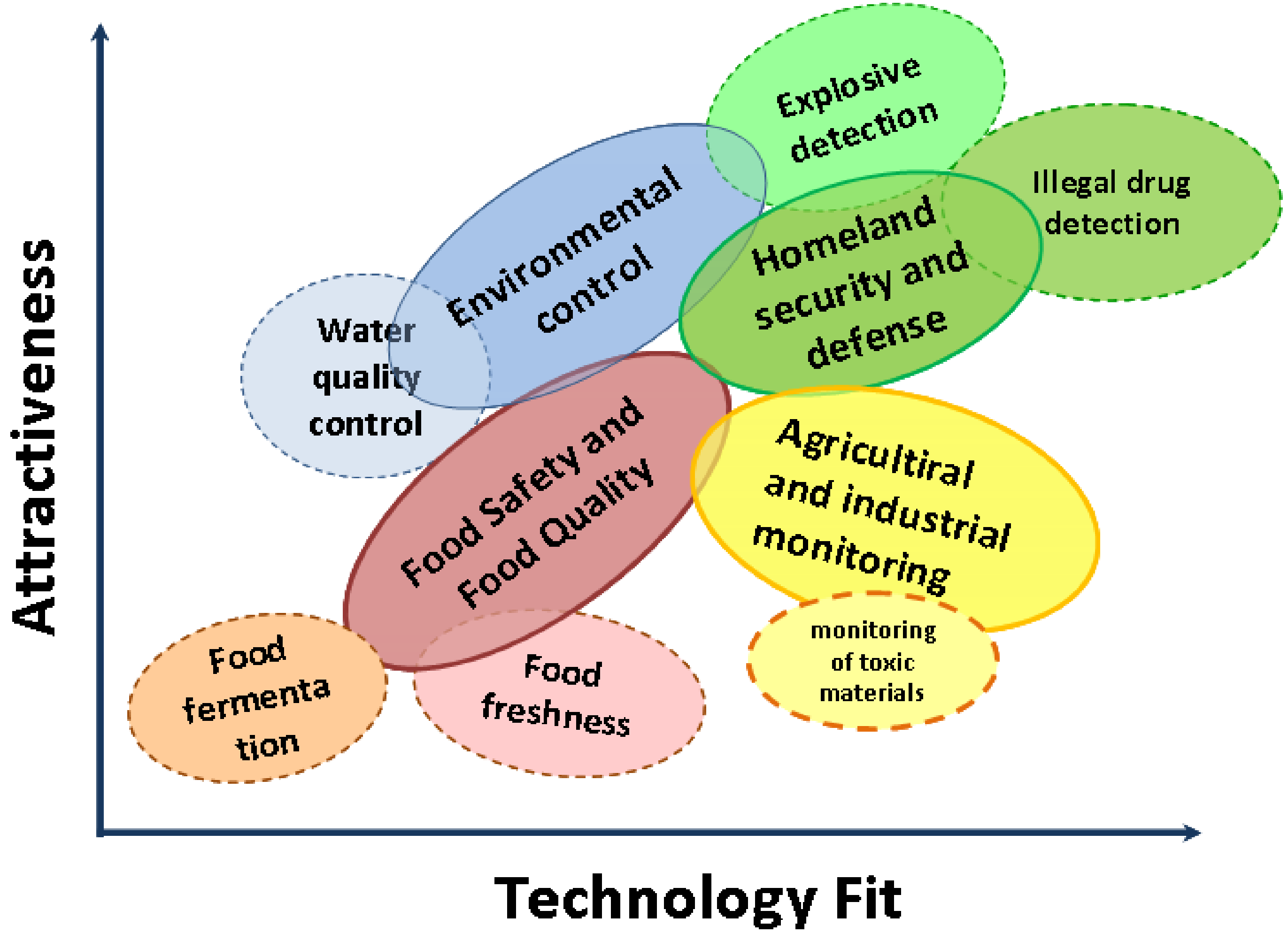


Figure 4: Conceptual design showing the sensor including the chip casette

CRIM-TRACK portable sensor unit containing:
chip cassette with multiple colorimetric chips, optics, electronics, power supply, wireless communication, interface to air sampler(s), etc.

Colorimetric Multi-sensor Technology Application Areas

1. Explosives detection
2. Detection of improvised explosives and their precursors
3. Illicit drug and drug precursor detection
4. Food freshness
5. Surveillance of industrial bioprocesses such as fermentation
6. Classification of indoor environmental quality
7. Water sources – classification of water quality
8. Diagnostics – exhaled breath



EXPERIMENTAL SETUP

CRIMTRACK prototype system

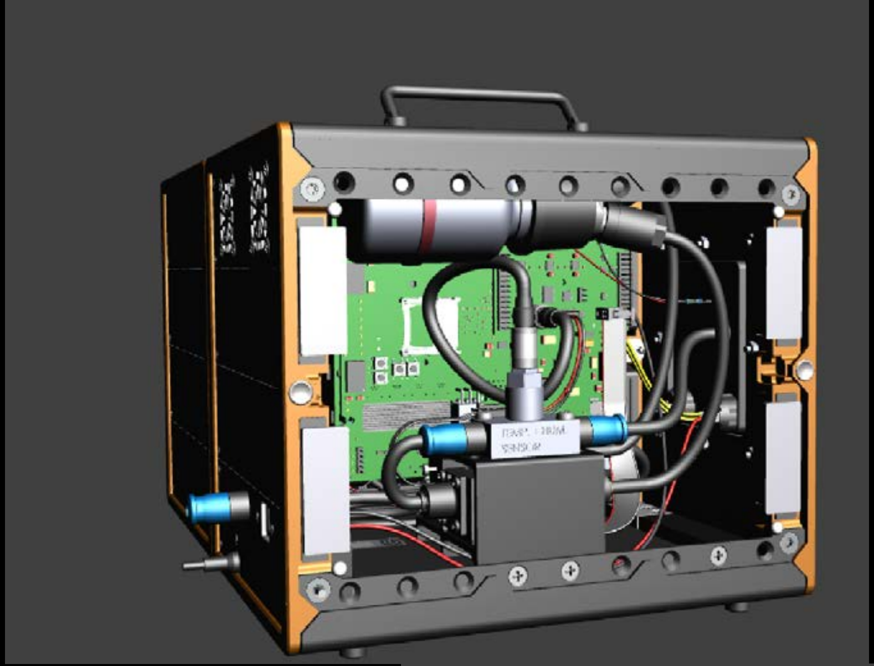
A portable & robust prototype. Based on modular housings with flexible I/O panels & mechanics. The flexible modular design allows easy adaptation to various test scenarios.

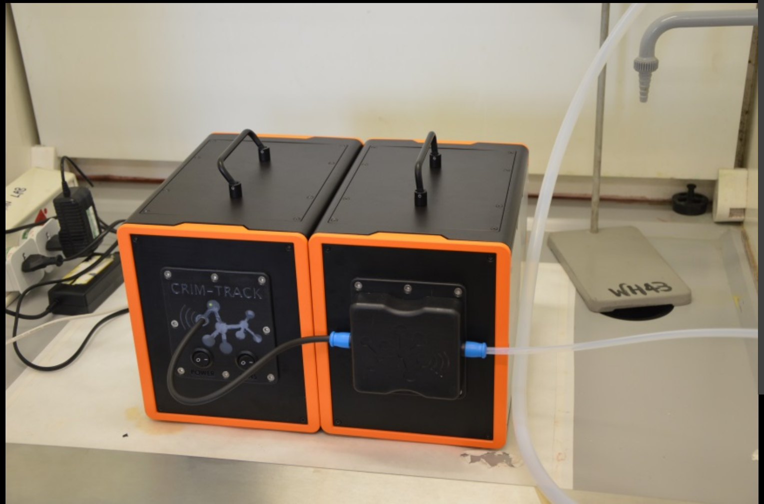
Left box contains pump, control board, and battery

Right box contains optics (camera), illumination, click-in slot for chip and flow chamber, control board, and battery.

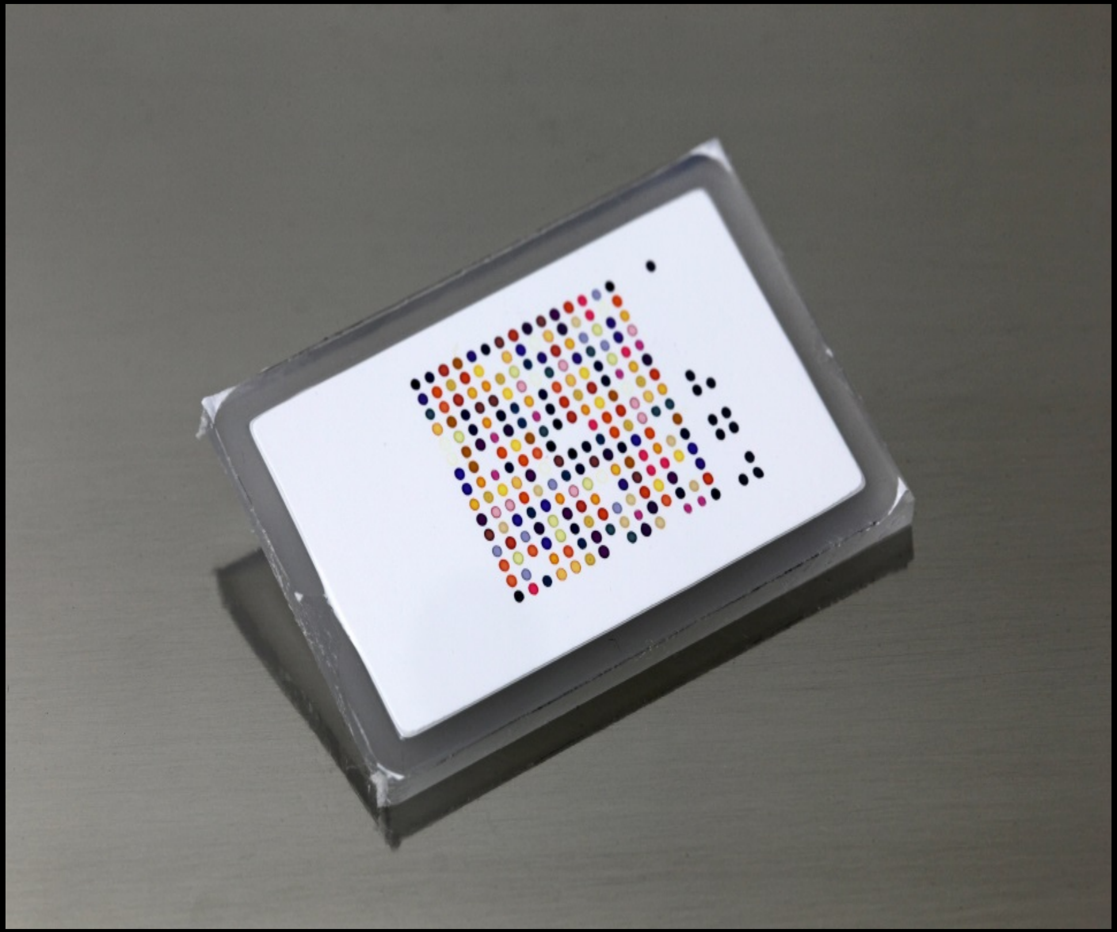
Can be operated either on battery alone or connected to mains power.

Includes flow, humidity, and temperature sensors.



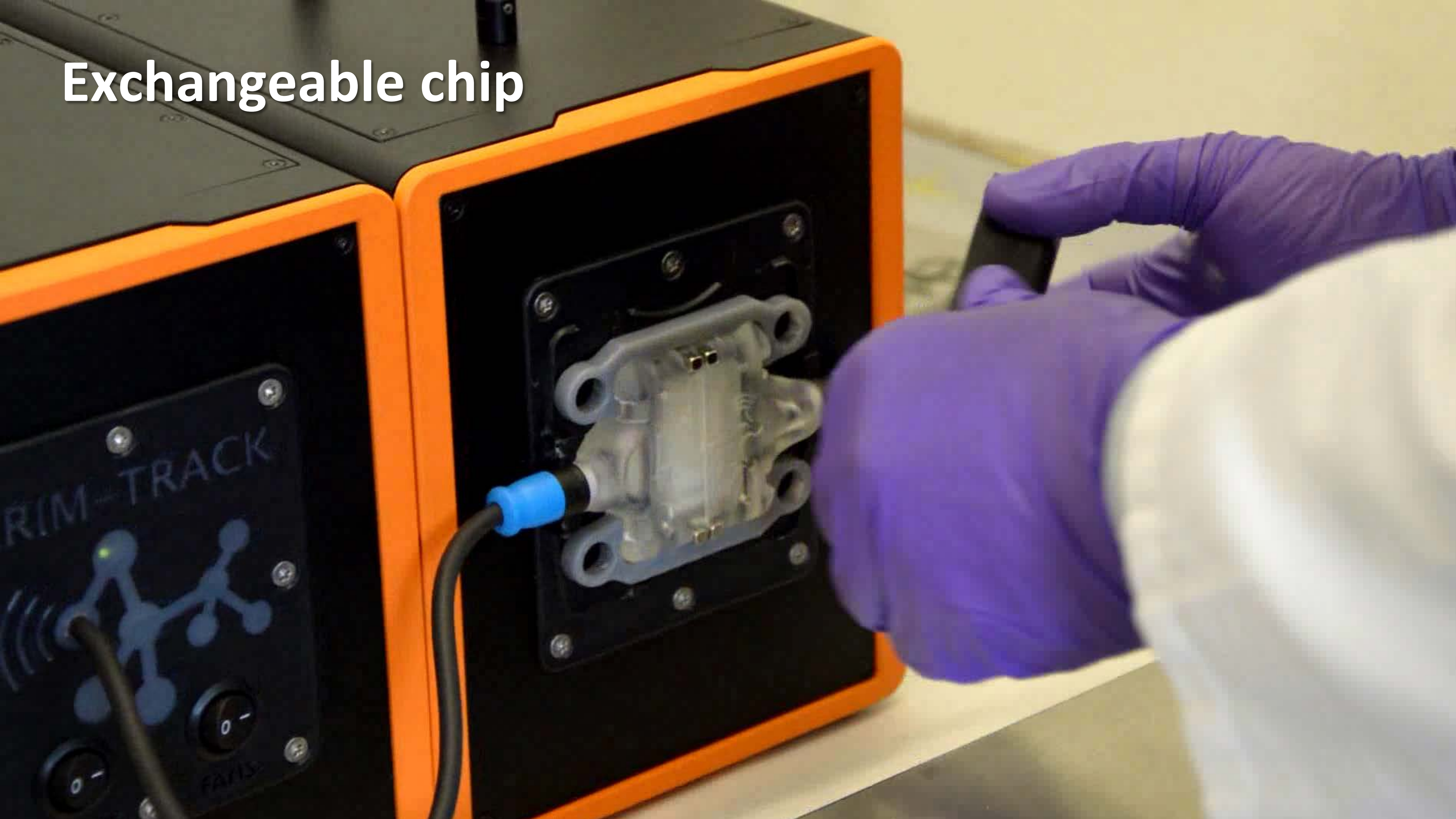


Disposable colorimetric chip



Chip layout: 15 x 15 array, 225 spots, 27 dyes in 8 replicates each, spot diameter 0.7 mm, centre – centre distance 1 mm

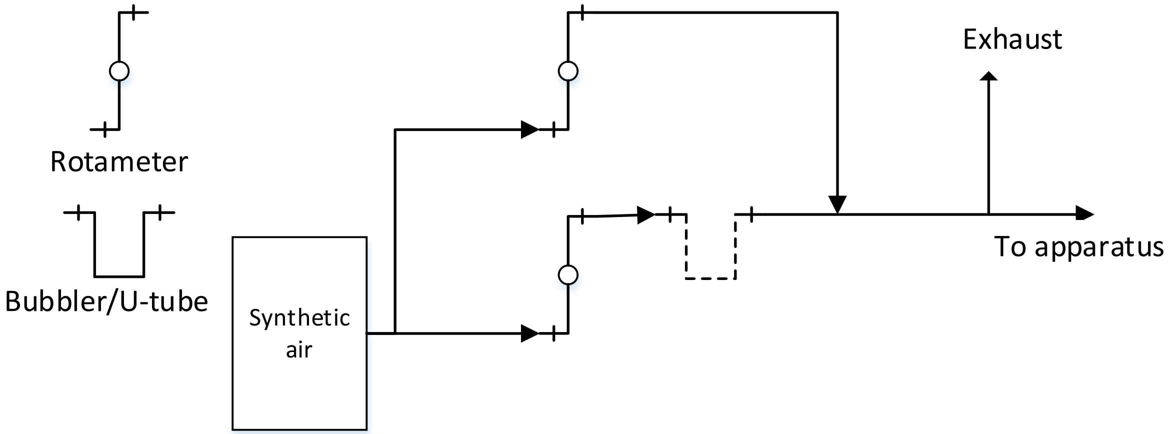
Exchangeable chip



Experimental setup - two target analytes are investigated

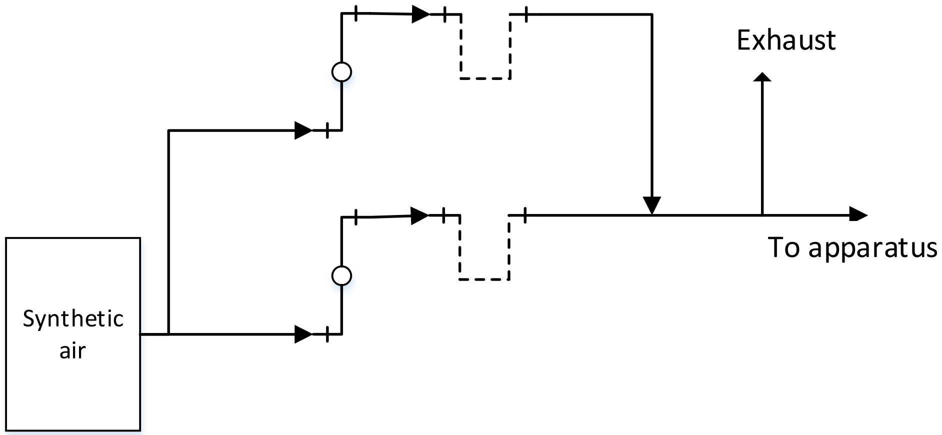
H_2O_2 - explosives precursor

- 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.



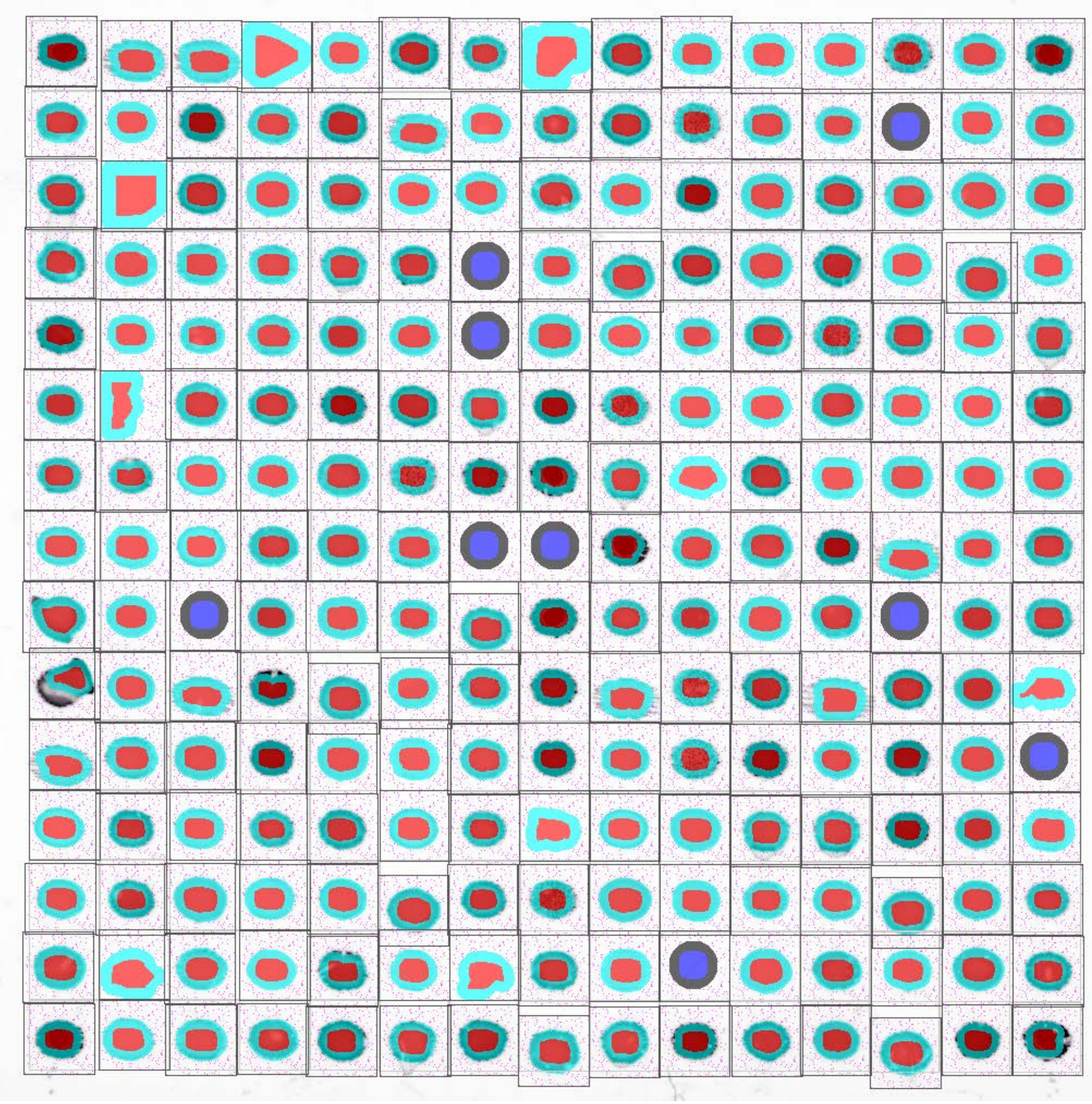
Sample generation

Glass gas washing bottle or Drechsel bottle with a glass frit. Used for liquid analytes and solutions.

Glass U-tube for liquid and solid samples. Inert glass fleece was optionally used to increase surface area.

DATA EXTRACTION

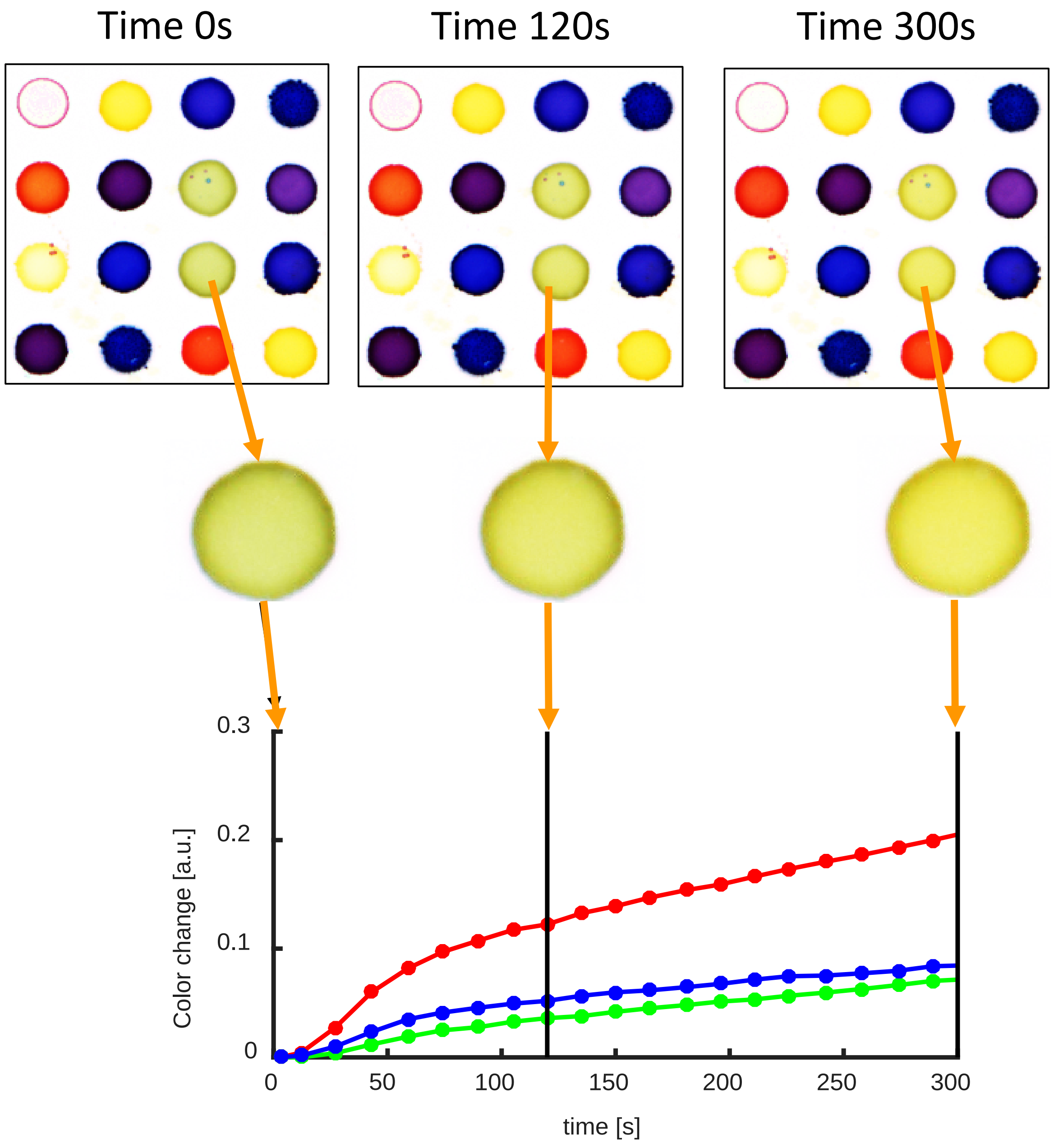
Data conditioning and preprocessing – median RGB values for each dye



Extraction of color change

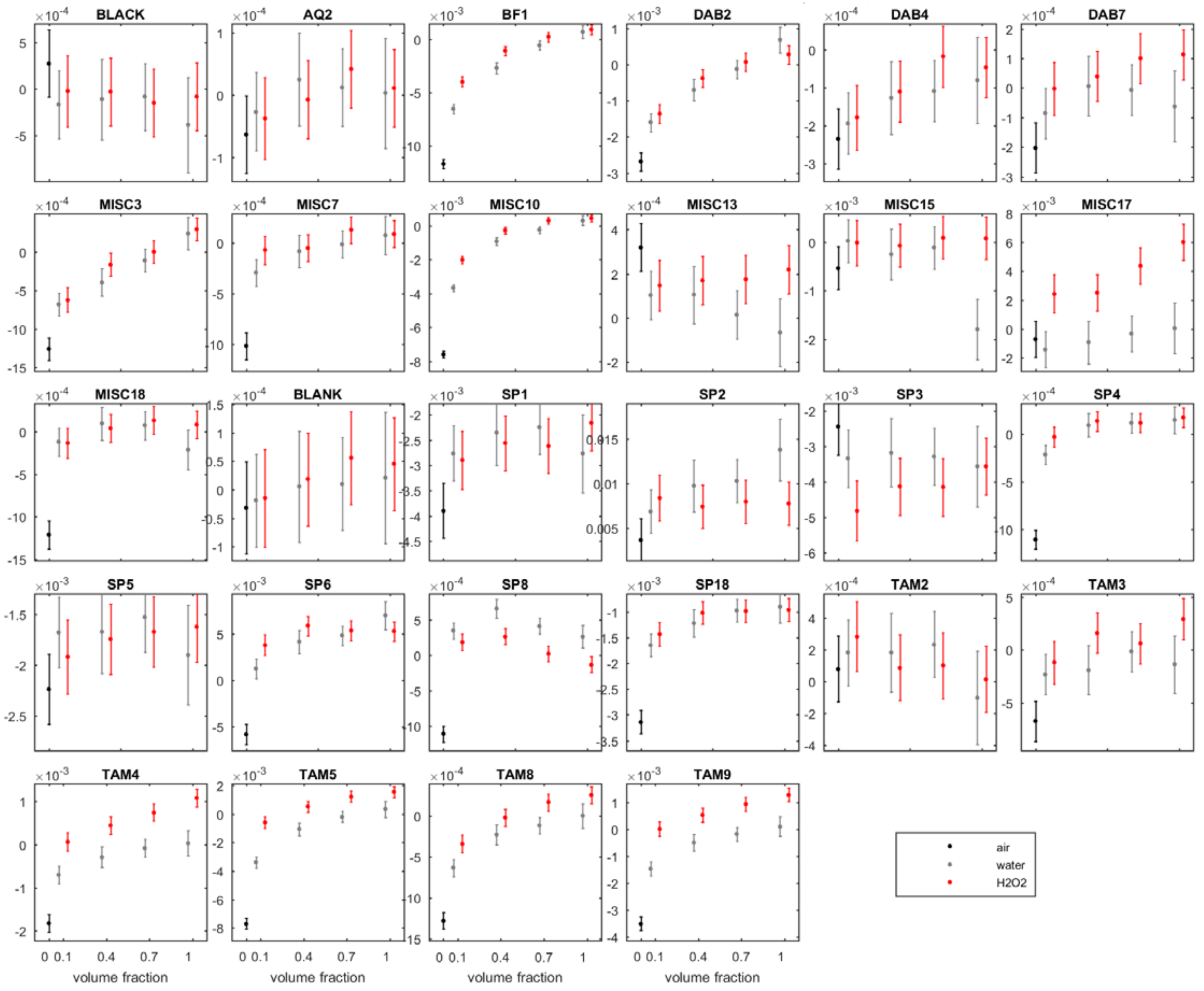
Dye spots are detected automatically and RGB color changes are summarized as the relative color change to the pre-image at 0s. The changes are small and requires sophisticated analysis.

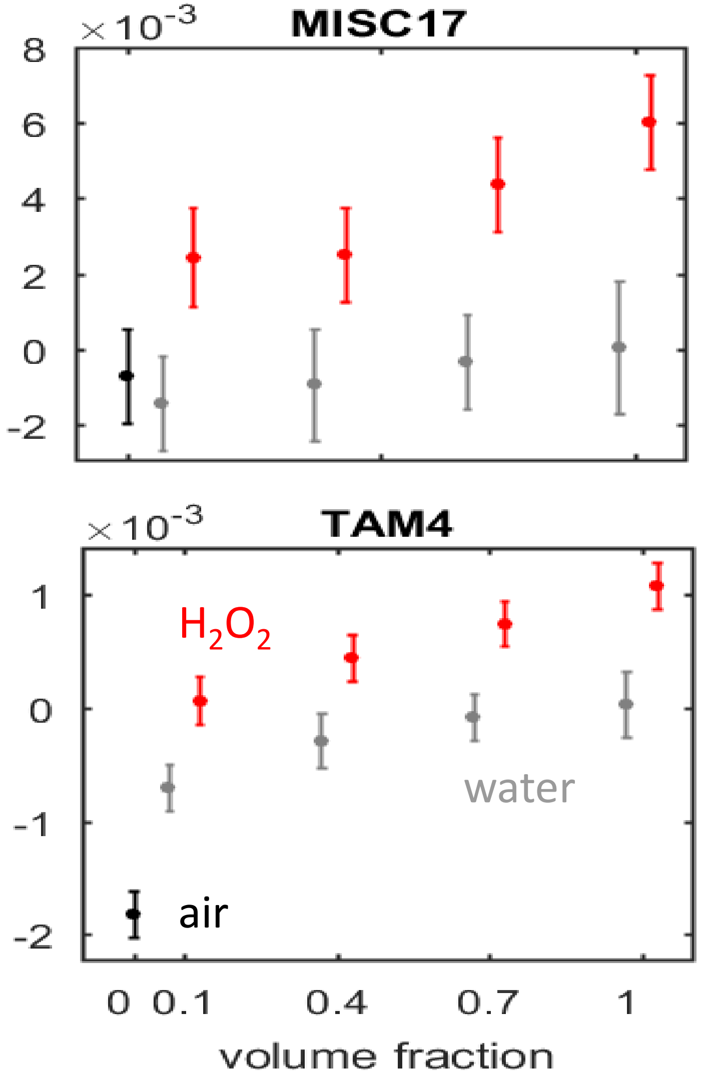
The color change is summarized by using the final color change after 5 minutes.



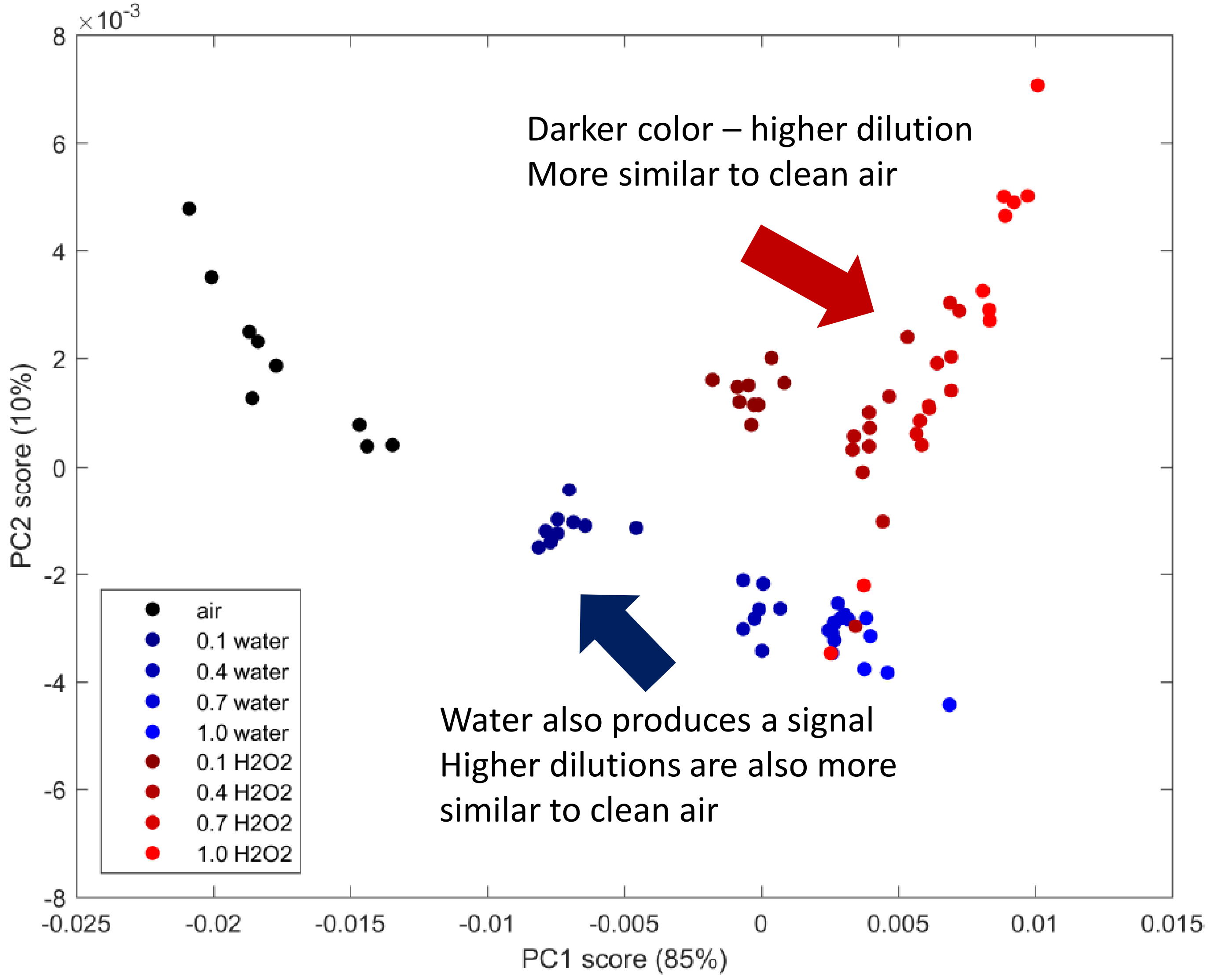
H_2O_2 dye color changes for dilution levels

Select dyes are good for detecting H_2O_2

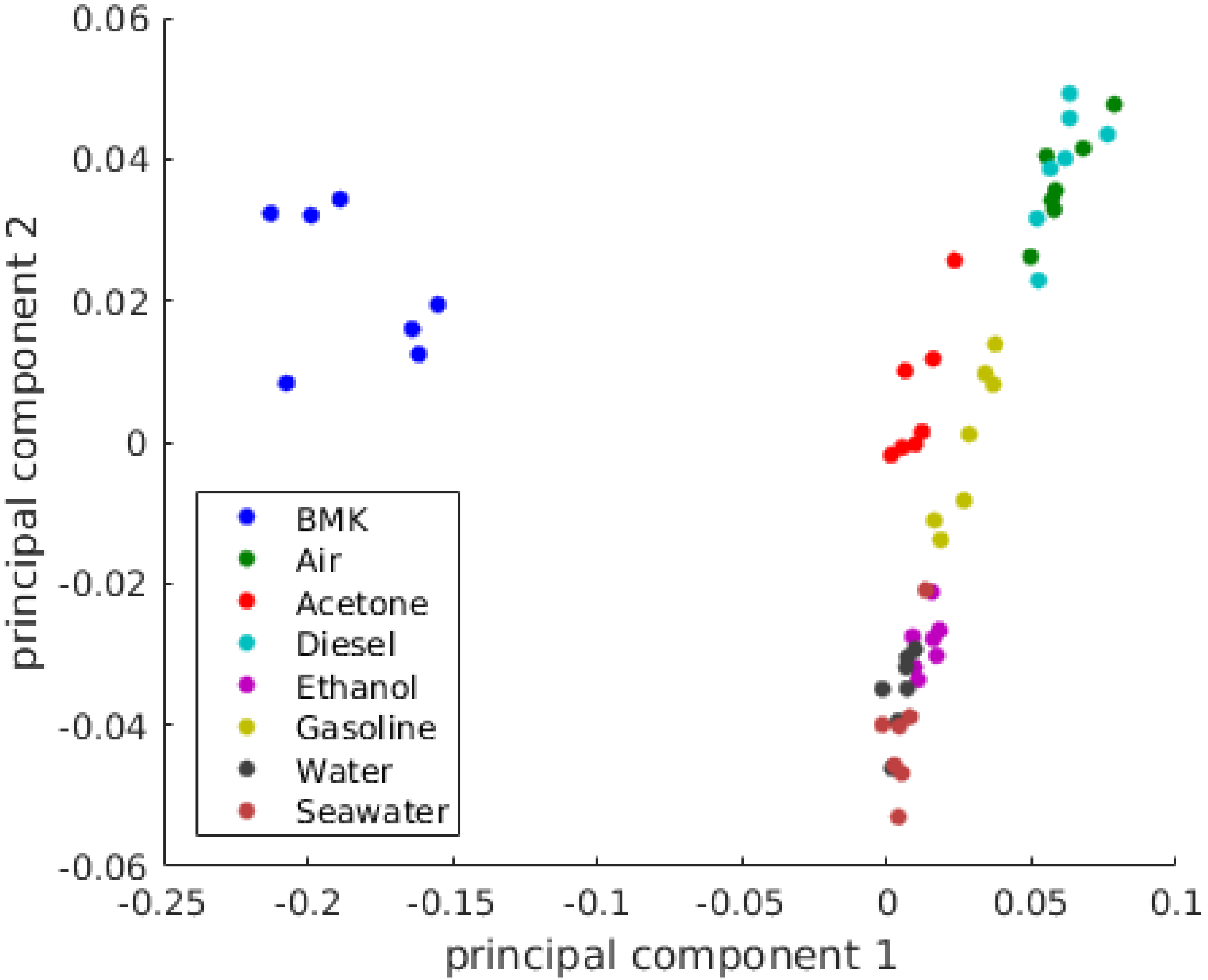




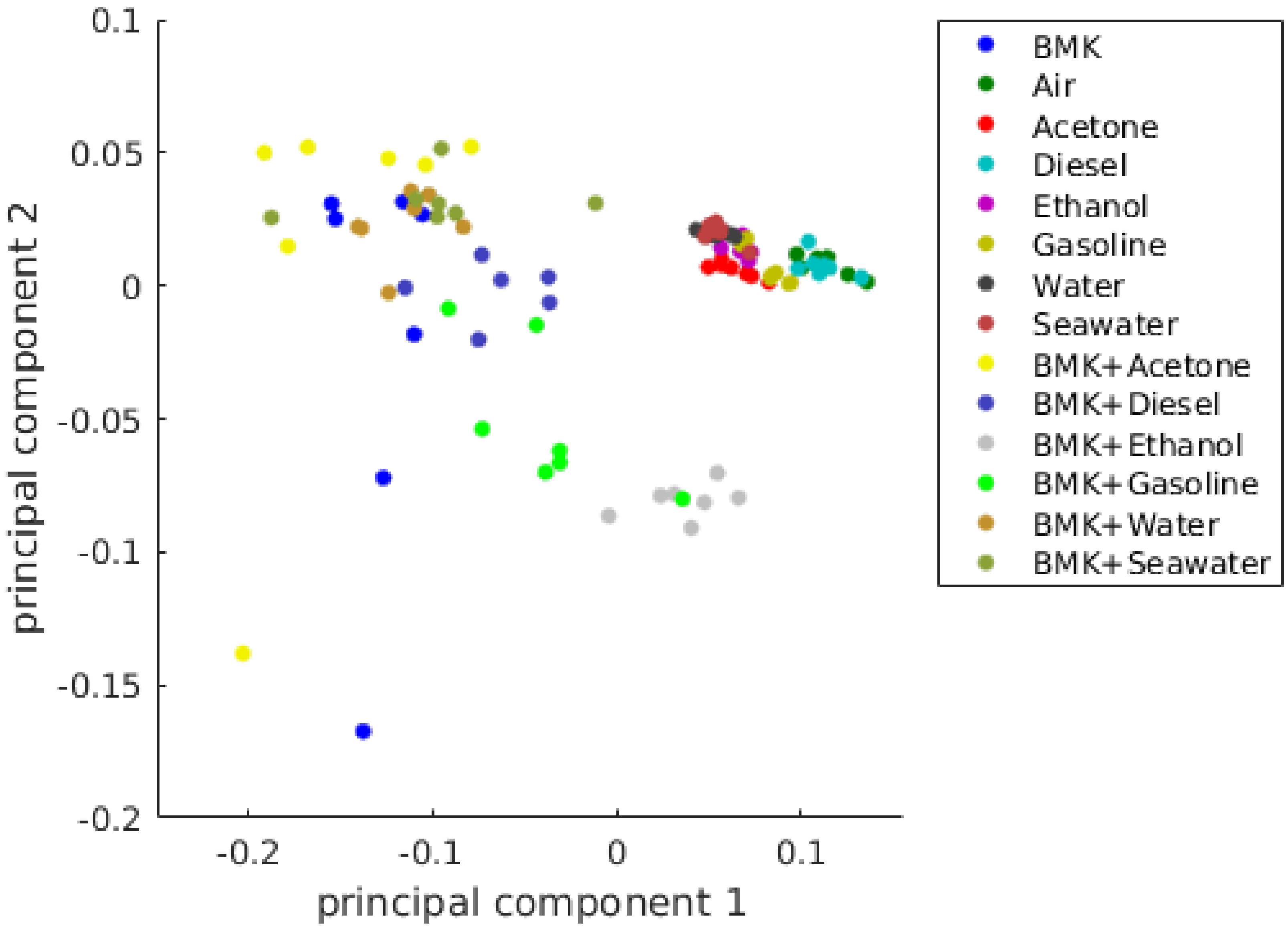
Principal Component Analysis based visualization – target is clearly separated



BMK samples PCA visualization



BMK samples PCA visualization



DETECTION RESULTS

Classification of H_20_2 – 10 fold cross-validation

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

KNN

True class	H_2O_2	confounder
H_2O_2	36	4
confounder	1	46

log.reg.

True class	H_2O_2	confounder
H_2O_2	39	1
confounder	20	27

RF

True class	H_2O_2	confounder
H_2O_2	38	2
confounder	2	45

Classification of BMK – 10 fold cross-validation

	KNN	logist. reg.	RF (no PCA)
clean BMK	97.3%	53.2%	100%
mixed BMK	100%	71%	100%
train clean/ test mixed	53%		86%

Conclusions

- The CRIM-TRACK fully-integrated prototype for air sampling has enabled the generation of standardized data.
- A data-driven machine learning approach to detect drug and explosives precursors using colorimetric sensor technology for air-sampling was successfully demonstrated.
- The experiments have demonstrated the possibility of detecting the target analytes in complex mixtures of confounding substance that occurs in real use cases.