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Automated identification of illicit substances by chemiometrics. Application to FTIR and RAMAN analysis.

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1. Context and motivation

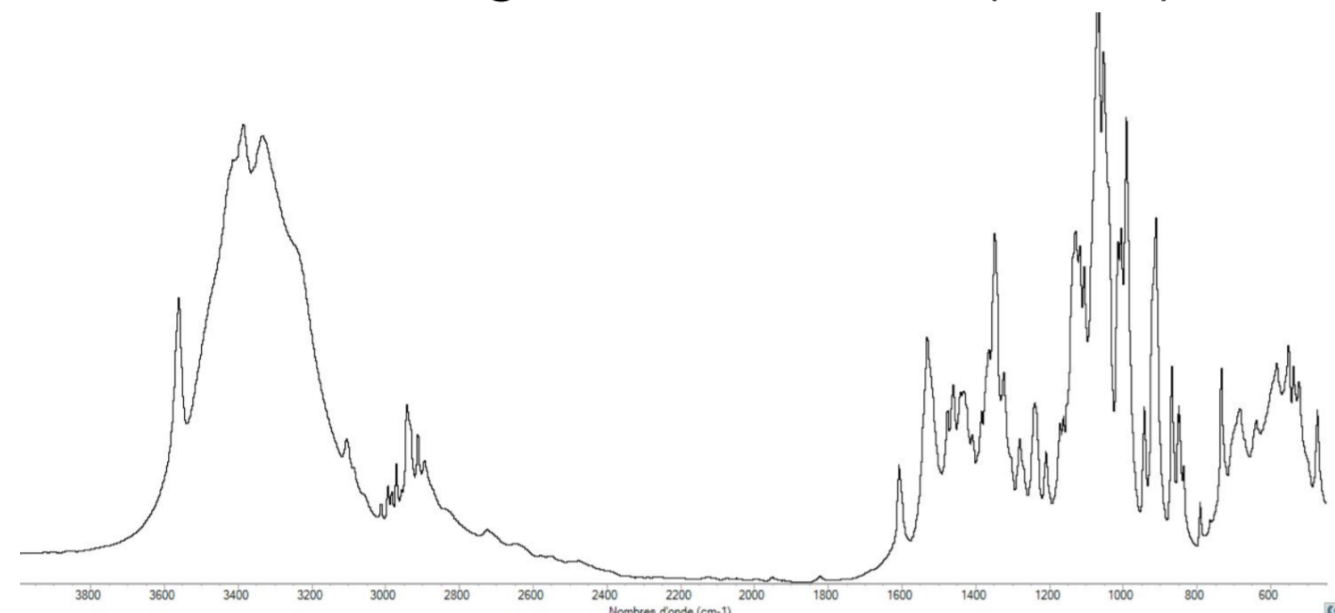
→ First steps of field investigation and analysis are largely based on robust and handheld analytical techniques such as FTIR or Raman spectrometry, etc. (fig. 1).

→ Removal of doubts is performed by comparing unknown spectra with reference spectra (database) and if necessary, cross-referencing the result of different analytical tools

→ Automated techniques currently in use are based on **spectral library searching with matching algorithms**.

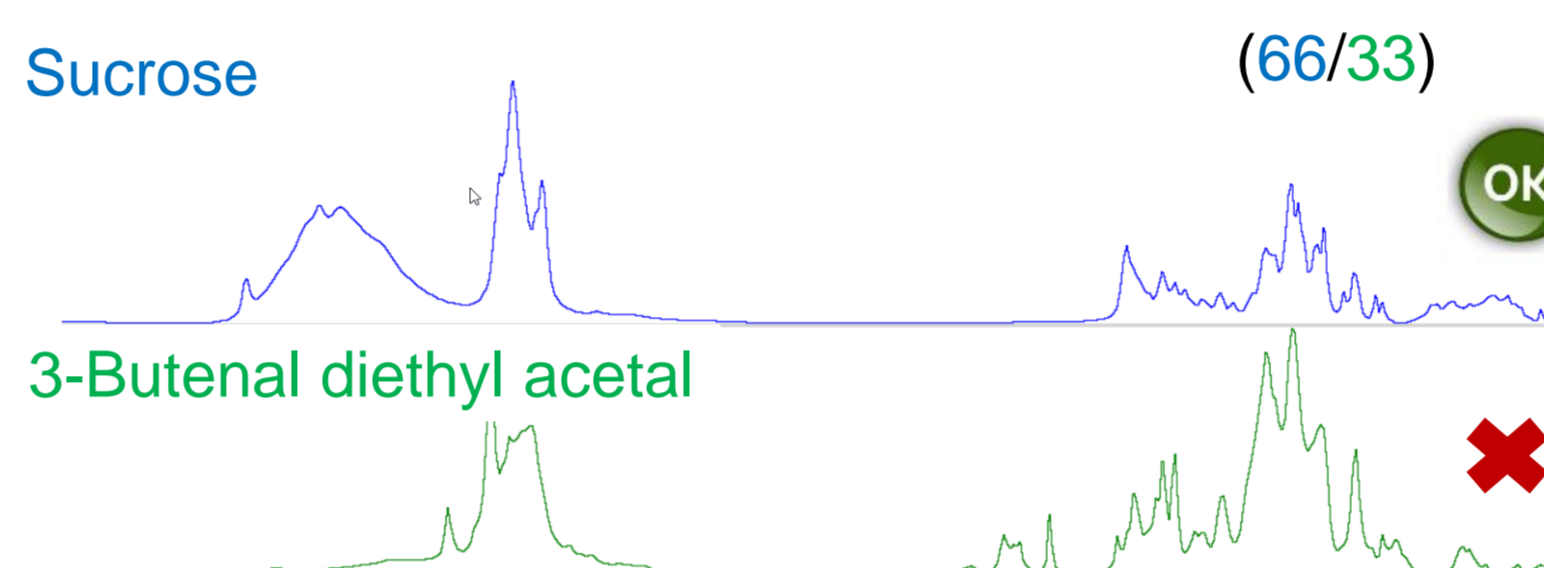
→ **These methods are limited** when searching target substances (drugs, explosives, chemical agent) in mixtures and even more if these substances are present in low concentrations.

Mixture of cane sugar and 2,4-DNT (88/22)



Correlation
Euclidean Distance
Absolute Value
1st Deriv Absolute Value
Least Squares
Correlation
1st Deriv Least Squares
1st Deriv Correlation

Example of spectral searching result



We propose hereafter a new approach based on training data generation (synthetic mixtures) and data separation algorithms to automatically identify threat signatures in unknown spectra

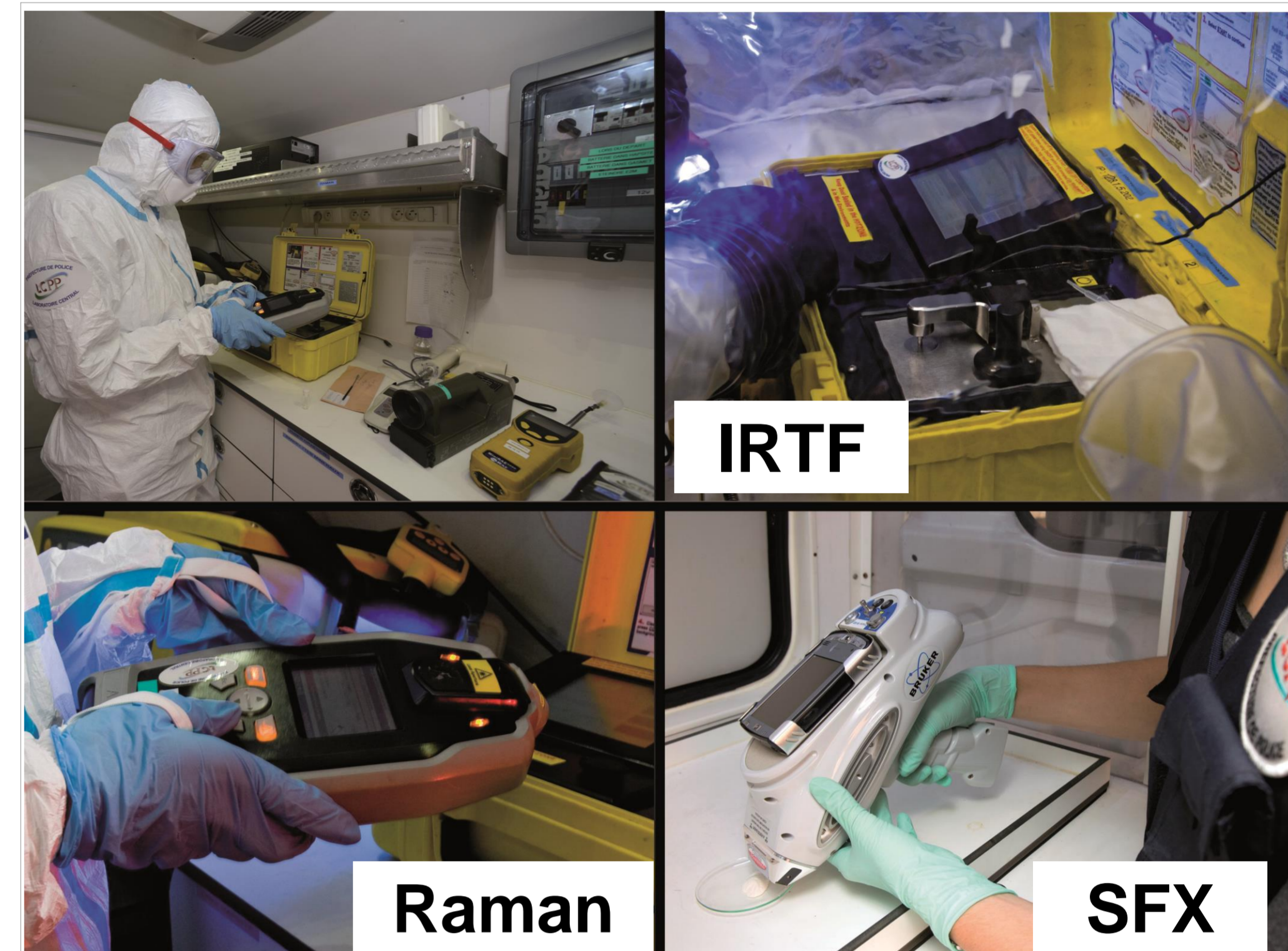


Figure 1 : Équipements analytiques du laboratoire mobile du Laboratoire central

© préfecture de police

2. Methodology and main achievements

Unknown spectra analysis
Automated Threat Identification

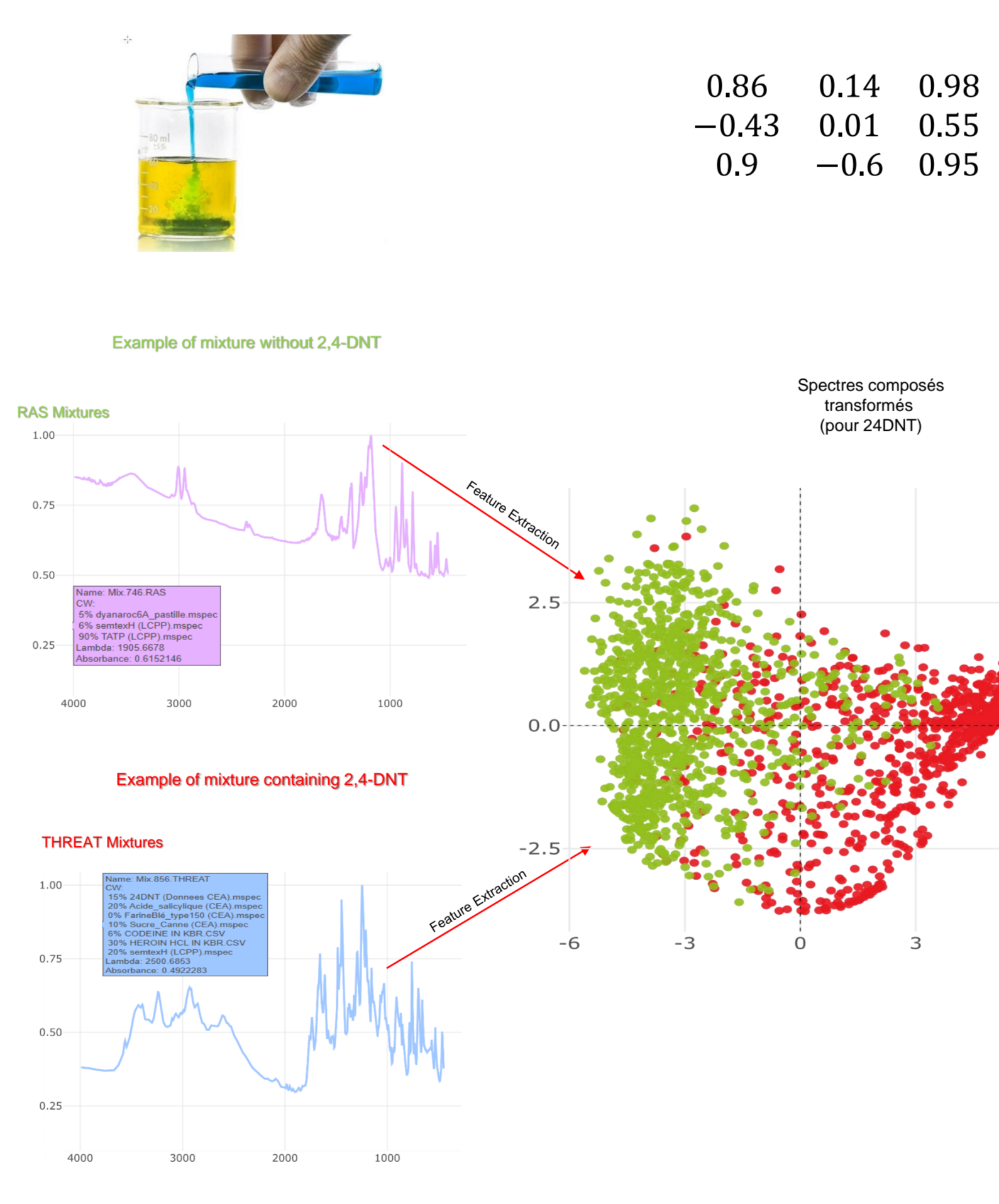
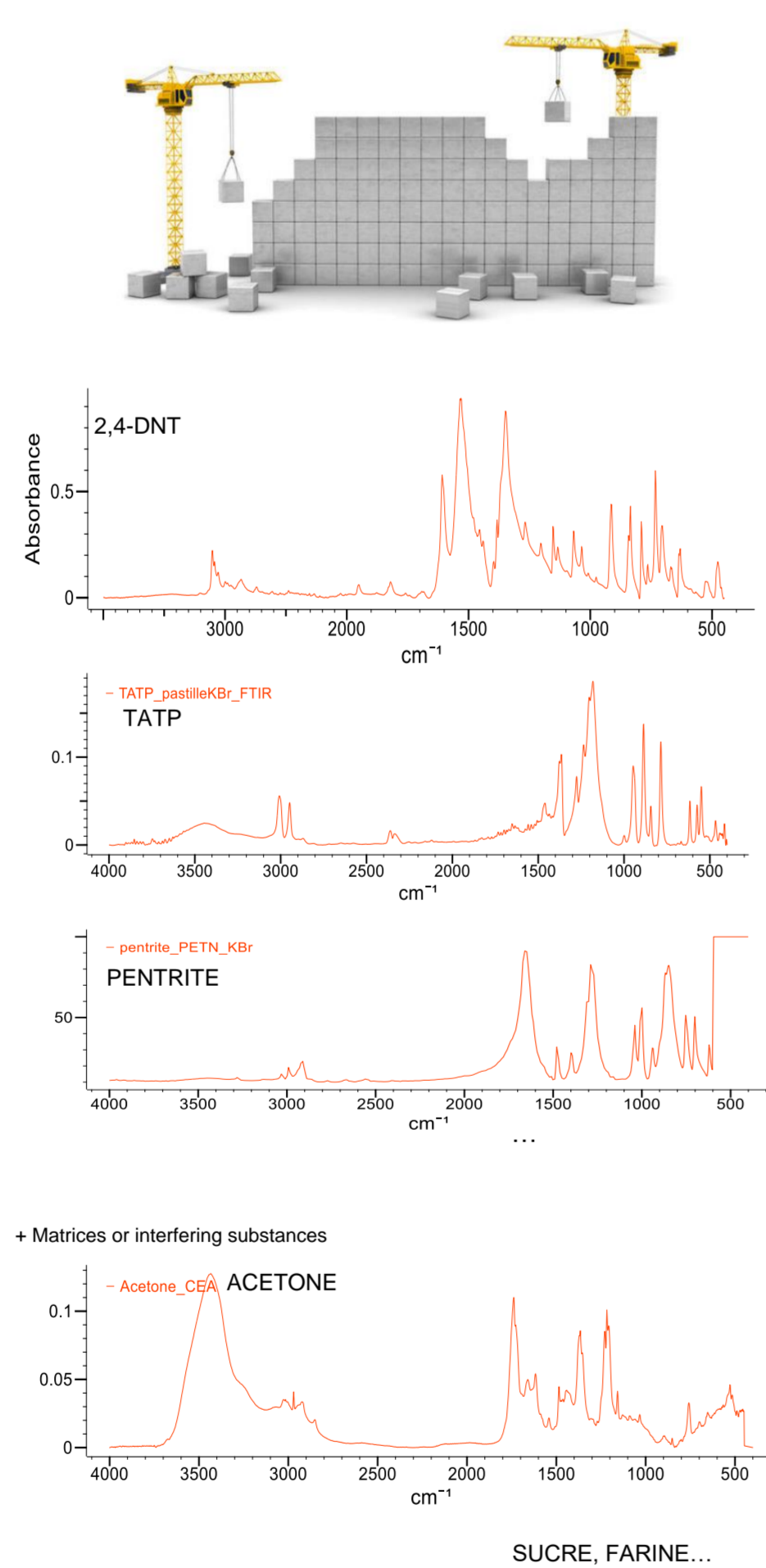
Compounds library

Synthetic mixtures generation

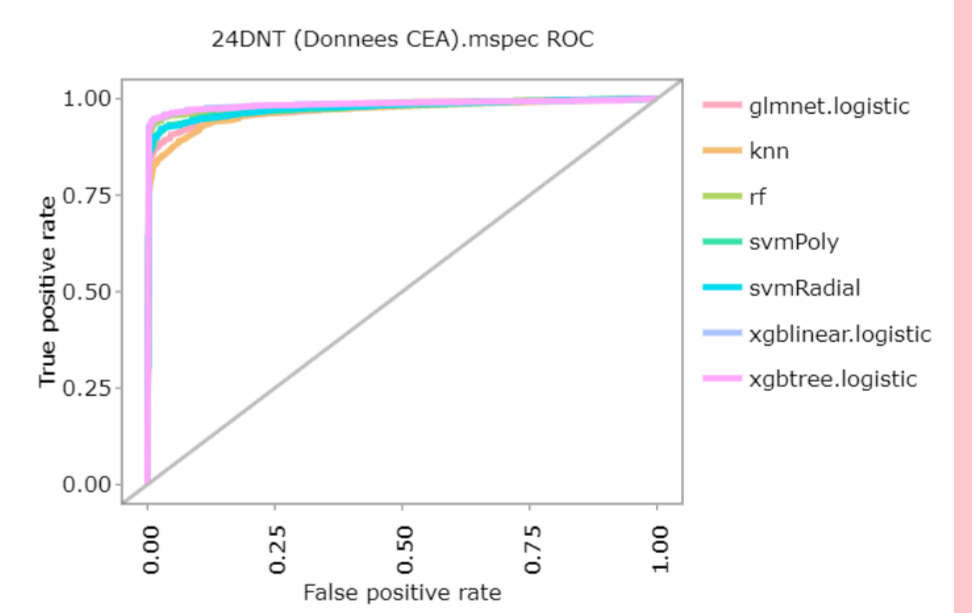
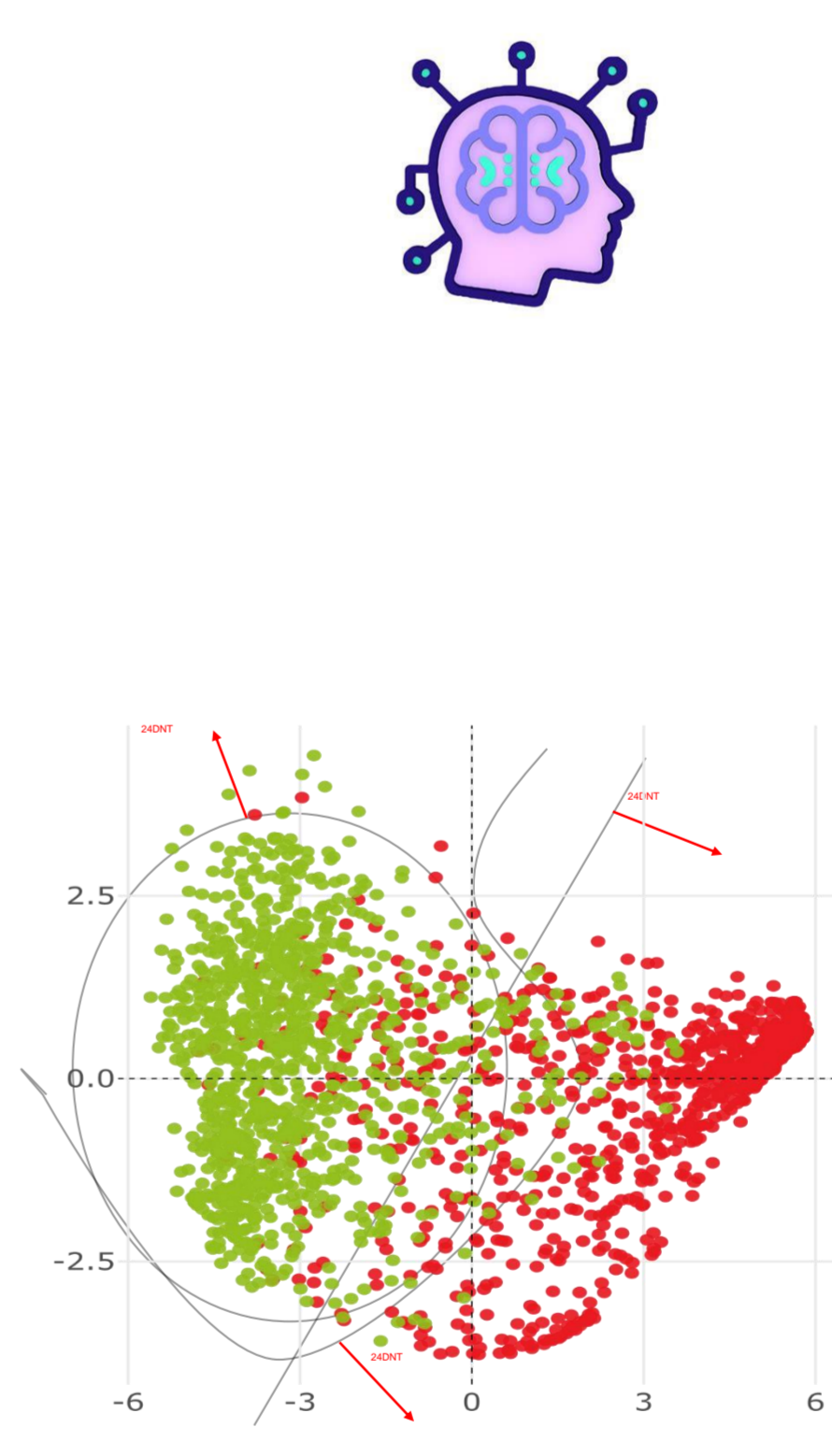
Features extraction

Models fitting

Models assessment



0.86 0.14 0.98
-0.43 0.01 0.55
0.9 -0.6 0.95



		Condition	
		THREAT	RAS
Prediction	THREAT	TP	FP
	RAS	FN	TN

$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{FP + TN}$$

3. Conclusions and Perspectives

The new tool under development allows the :

- generation of complex mixtures parametrized by 3 variables and a noise.
- training of different models
- performance assessments of the different supervised learning algorithms
 - on synthetic mixtures (200 inputs min), complex mixtures (quaternary mixtures on average)
 - at different concentrations of the target threat
 - on real spectra (pure threats/interfering substances and unknown mixtures)

These new algorithms are compatible with different analytical techniques that could be combined to improve decision making process.

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