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

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AUTOMATED IDENTIFICATION OF ILLICIT SUBSTANCES BY CHEMIOMETRICS. APPLICATION TO FTIR AND RAMAN ANALYSIS

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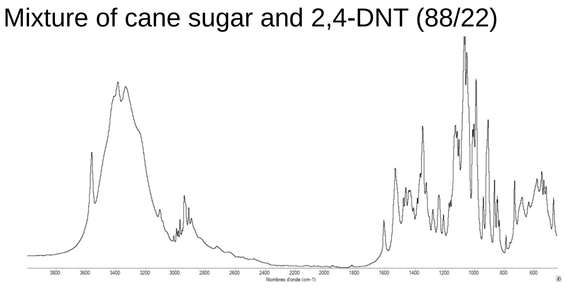
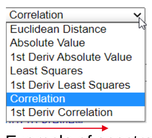
1. Context and motivation

→ 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.

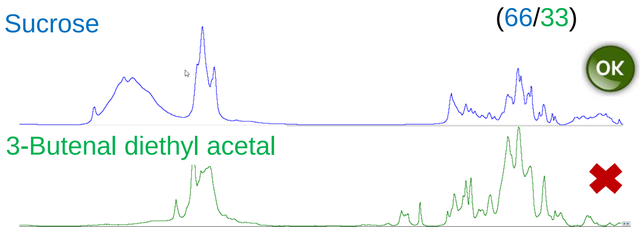
Mixture of cane sugar and 2,4-DNT (88/22)





Example of spectral searching result

Sucrose (66/33)



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

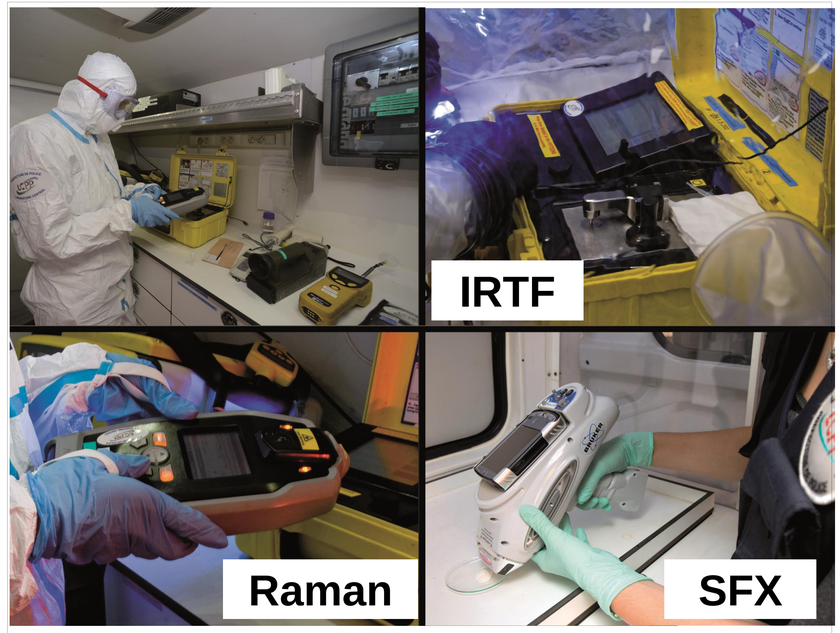


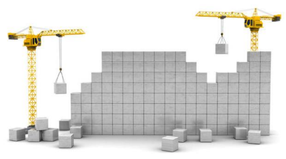
Figure 1 : *Équipements analytiques du laboratoire mobile du Laboratoire central* *© préfecture de police*

2. Methodology and main achievements

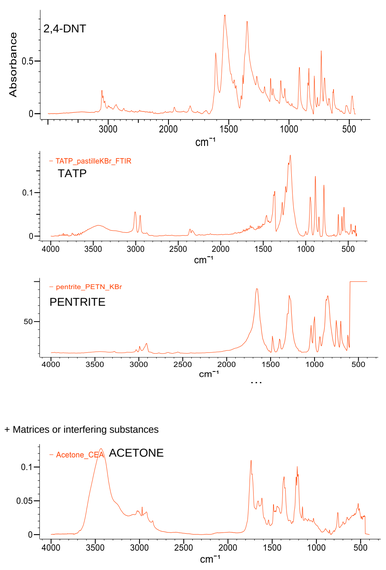
Unknown spectra analysis

Automated Threat Identification

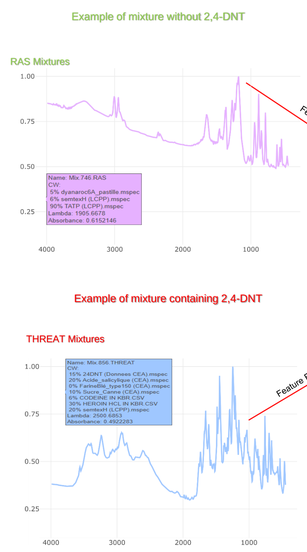
Compounds library | Synthetic mixtures generation | Features extraction | Models fitting | Models assessment

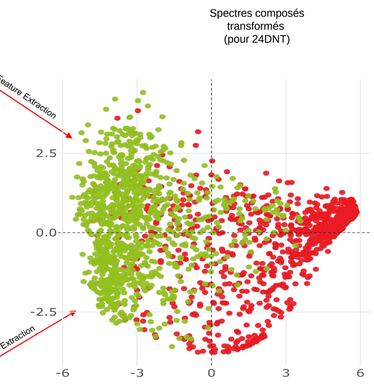


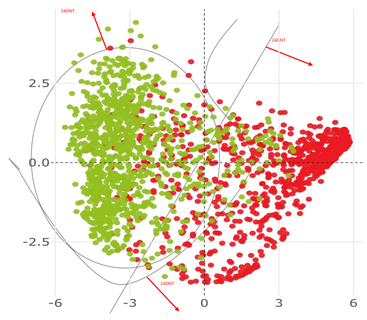
$$\begin{matrix} 0.86 & 0.14 & 0.98 \\ -0.43 & 0.01 & 0.55 \\ 0.9 & -0.6 & 0.95 \end{matrix}$$



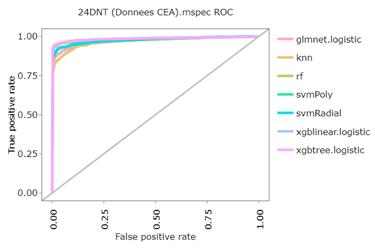
SUCRE, FARINE…







Diversity of models (extendable)
- ✓ SVM
- ✓ kNN
- ✓ GLMs
- ✓ Random Forest
- ✓ *Gradient boosting*

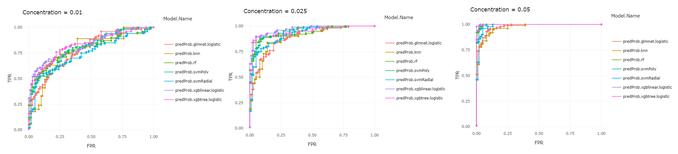


		Condition	
		THREAT	RAS
Prédiction	THREAT	*TP*	*FP*
	RAS	*FN*	*TN*

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

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

Complexity of synthetic mixes
1. Compounds.per.mix.expected = 4
2. Abundance.profile.expected = 2
3. Target.threat.presence.probability = 0.4
4. Number.of.mixtures = 1000



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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