TWO-STAGE SYNTHETIC DRUGS DISCRIMINATION IN BLOTTER PAPERS BY MIR SPECTROSCOPY AND PLS-DA

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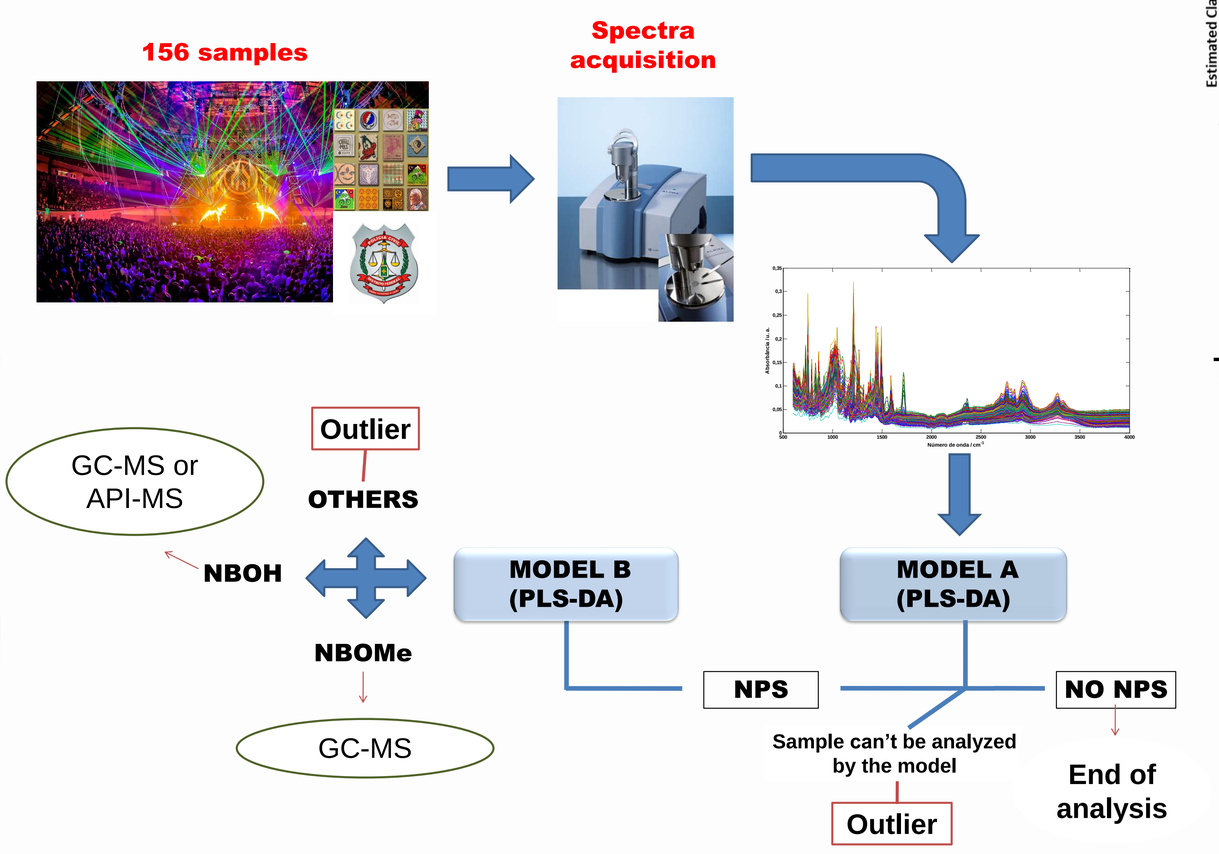
Introduction and Objective

- Blotter paper seizures containing new psychoactive substances (NPS) such as NBOMe and NBOH are increasing over the last years.
- Usually blotter paper analysis is performed by GC-MS.
- NBOH compounds need an ambient ionization or a modified GC-MS method to avoid misidentification with 2C-I.[1]
- Spectroscopic methods such as ATR-FTIR associated to PLS-DA are an alternative for a rapid sceening of NPS in blotter papers.

➢ The objective of this work is the development of a two-stage discrimination method for NPS in blotter papers using ATR-FTIR and PLS-DA.

Methods



Results

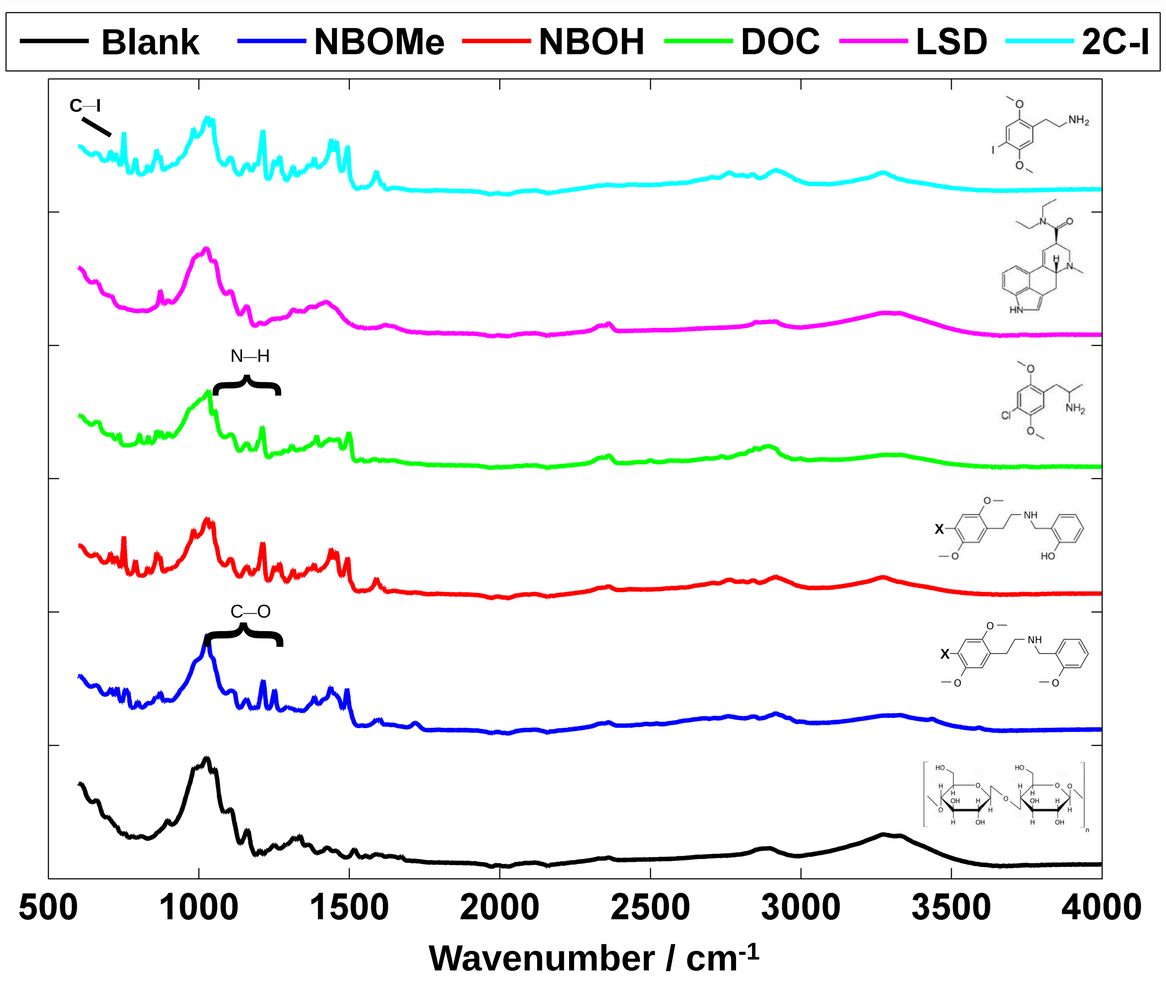


Figure 1. Characteristic spectra of blank and studied substances.

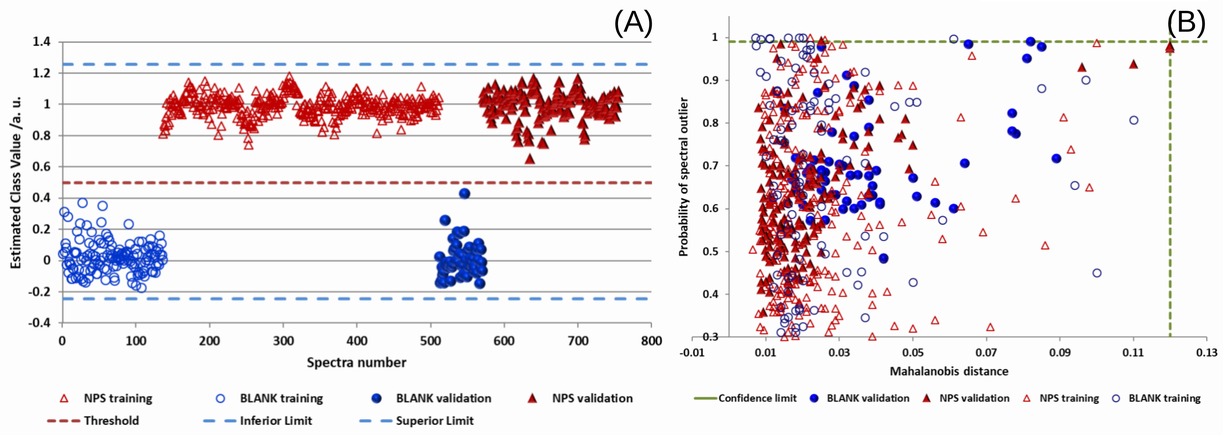


Figure 2. (A) Estimated class values and (B) spectral residual probability versus Mahalanobis distance for Model A.

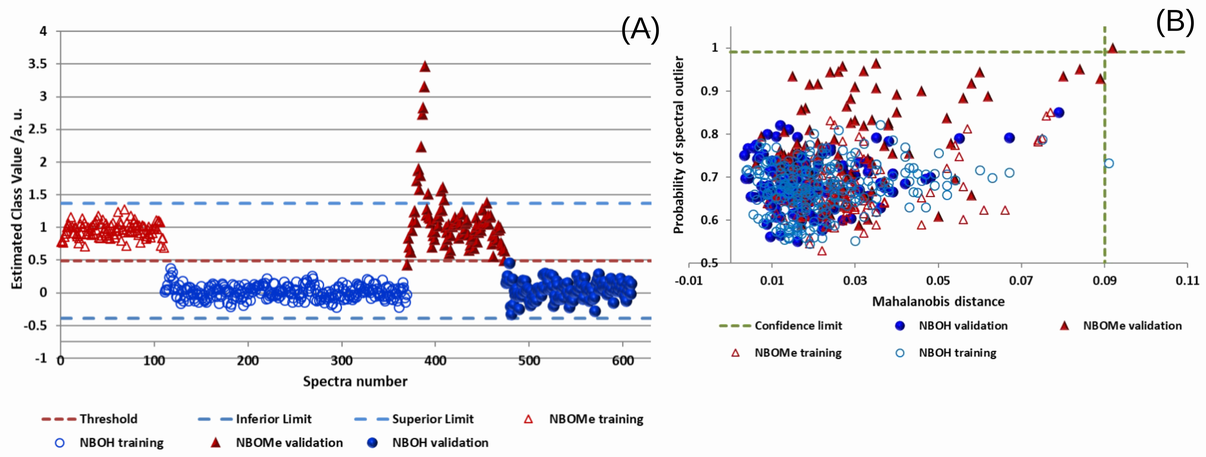


Figure 3. (A) Estimated class values and **(B)** spectral residual probability versus Mahalanobis distance for Model B.

Table 1. Figures of merit for models A and B.

MODEL A – 13 latent variables				
Phase	**Class**	**FPR (%)**	**FNR (%)**	**EFR (%)**
Training	No NPS	0	0	100
	NPS	0	0	100
Validation	No NPS	0	0	100
	NPS	0	0	100
MODEL B – 9 latent variables				
Fase	**Class**	**FPR (%)**	**FNR (%)**	**EFR (%)**
Training	NBOMe	0	0	100
	NBOH	0	0	100
Validation	NBOMe	0	0	100
	NBOH	0	0	100

FPR - False positive rate FNR - False negative rate EFR – Efficiency rate.

Conclusions

- This is a cheap and fast non-destructive procedure, which requires no sample preparation and can be performed in less than ten minutes in a standard ATR-FTIR.
- The proposed method presented efficiency rates of 100% and can be easily updated to include new drugs or drug classes.[2]
- Outliers are rapidly identified considering superior and inferior limits as well as Mahalanobis distance and spectral residual probability.
- The proposed method can be used as a blotter paper screening routine in forensic laboratories.

References

[1] Arantes, L.C.; Ferrari Júnior, E.; Souza, L.F.; Cardoso, A.C.; Alcântara, T.L.F.; Lião, L.M.; Machado, Y.; Lordeiro, R.A.; Coelho Neto, J.; Andrade, A.F.B. *Forensic Toxicol*. 35 (2017) 408-414. doi: 10.1007/s11419-017-0357-x.

[2] Pereira, L.S.A.; Lisboa, F.L.C.; Coelho Neto, J.; Valladão, F.; Sena, M. *Microchem. J.* 133 (2017) 96–103. doi:10.1016/j.microc.2017.03.032.

Acknowledgments

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