

Rapid field identification of illicit drugs based on electroanalysis assisted by machine learning

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Trafficking and consumption of illicit drugs have become a well-known worldwide burden over the last years [1, 2]. Not only from a health (physical & mental effects) and economical point of view, but also due to their consequences in the society (e.g. existence of drug mafias and drug dealers, increase in violence, traffic, underground economy, etc.). In order to be able to dismantle such fraudulent activities and safeguard the public, security and law enforcement agencies require of fast and portable methods that allow them to reliably achieve the identification of drugs upon its interception. However, the rapid detection of illicit drugs is still challenging, especially when facing the on-site analysis [3].

In this regard, electrochemical sensors offer fast and accurate information in a cost-effective manner, being highly suitable for the development of compact and user-friendly hand-held meters for on-site analysis due to their minimal power requirement, potential for miniaturization and portability, low-cost instrumentation or ease of operation, between other advantages [4]. These features have been stressed with the emergence of additive manufacturing (most commonly known as 3D printing) as an alternative approach for the fabrication of customized electrochemical sensors, owing to advantages such as low-cost (both of the material and equipment), tunability and easy prototyping [5,6]. Concretely, electrodes are fabricated by fused deposition modelling (FDM) from thermoplastics such as polylactic acid (PLA) or acrylonitrile-butadiene-styrene (ABS), commonly doped with different carbon-based materials such as carbon black, carbon nanotubes (CNTs) or graphene to overcome the insulating nature of PLA and ABS.

However, despite the inherent redox activity of most of the drugs, which makes possible their identification by using electrochemical sensors, the simultaneous determination of seized samples might still be challenging given the complexity of the intercepts and the similar electrochemical response of some drugs and usual cutting agents. Precisely, one of the main drawbacks faced is the possible overlapping between peaks when mixtures of those are analyzed, which can even lead to the suppression of some peaks [7]. In this direction, the coupling of electrochemical sensors with machine learning or artificial intelligence (AI) modelling allows identifying the illicit drug fingerprint from these

complex data. Thus, with such an approach it is possible to deconvolute complex overlapping electrochemical responses and achieve the simultaneous identification and quantification of drugs plus cutting agents. Moreover, the use of an array of chemically-modified sensors, rather than relying on a single bare electrode can also further improve the potential of the system; an approach that is known as electronic tongue (ET) [8,9].

In this direction, herein we present an overview of some of the achievements made so far in the detection of illicit drugs and some of their common cutting agents, using both commercial and 3D-printed electrochemical sensors (Figure 1). Given the complexity of the scenario, the analysis with commercial electrodes has been taken as testbed to demonstrate the potential of the approach, with a series of experiments planned in increasing order of complexity, covering from initial qualitative experiments (Figure 2) to the quantitative identification of different drugs mixtures (Figure 3), both in the absence and presences of different cutting agents.

Overall, the combination of modified voltammetric sensors with different machine learning algorithms has proven to be a useful approach for the analysis of drugs. A very satisfactory performance has been obtained both in the qualitative discrimination of different substances or in its simultaneous quantification, even when mixed with other drugs and/or different cutting agents. More importantly, the reported approach herein demonstrates the potential of 3D-printing as a viable option for the preparation of customized voltammetric sensors, with many added advantages as are the automation, simplicity and low cost of both the system and the materials. Furthermore, the versatility and high-adaptability of the design combined with the excellent performance of the material have to be highlighted. Consequently, taking into account the performance demonstrated herein and the inherent advantages of electrochemical methods such as its simplicity, low-cost and portability, the suitability of the current approach for the development of portable system for decentralized analysis is confirmed.

References

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Figures

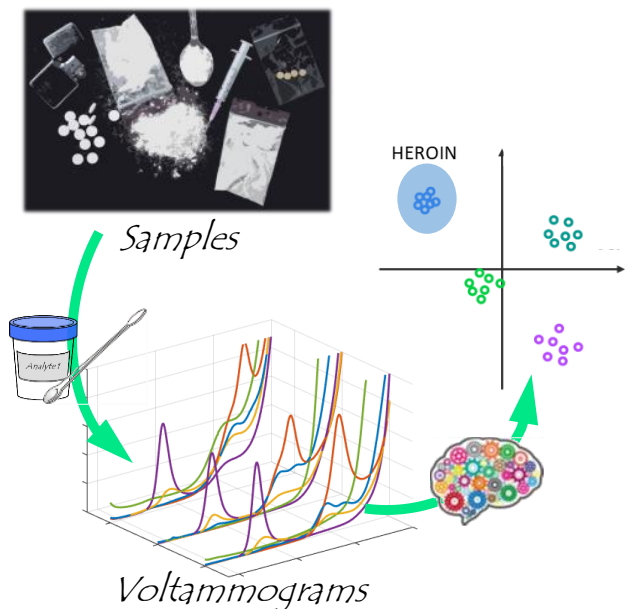


Figure 1. Schematic of the proposed approach for the identification and quantification of illicit drugs in seized samples.

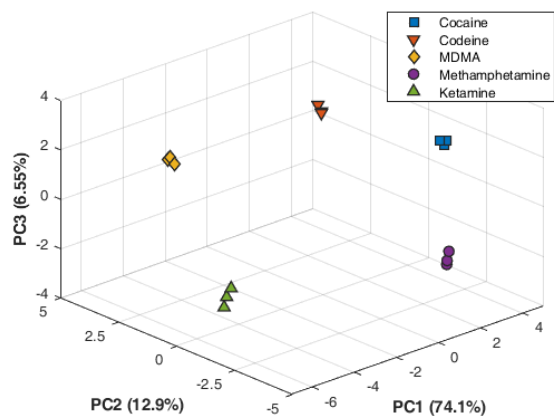


Figure 2. Score plot obtained from the principal component analysis of the voltammetric responses of different drugs.

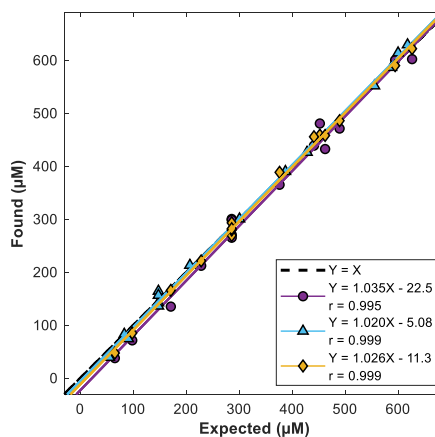


Figure 3. Modelling ability of the genetic algorithms-partial least squares regression (GA-PLS) model for the quantification of (●) heroin, (▲) morphine and (◆) codeine mixtures in the range 0-700 µM. Set adjustments of obtained vs. expected concentrations for the test subset. Additionally, the ideal comparison line (y=x) is also plotted.