B146 The Easy Application of Chemometrics to Forensic Chemical Data: A Software Tool for Forensic Chemists

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Learning Overview: The goal of this presentation is to inform attendees about a free specialized software being developed in Europe that facilitates easier application of chemometric methods in forensic chemistry casework, such as classification or profiling of drugs.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by introducing a new software tool that allows easy application of the chemometric methods most commonly found in literature to real casework involving chemical data.

In recent years, chemometric methods have been explored to help analyze and extract useful information from forensic chemical data. While these methods have seen some success, their utilization usually requires rather advanced statistical and data analysis skills, such as deep theoretical understanding of statistics and statistical software. For this reason, the application of these methods can be intimidating for many forensic chemists, despite the clear benefits they could provide. To help resolve this issue, a specialized and free software called ChemoRe is being developed in Europe.

The work on ChemoRe was started in 2018 as the European Network of Forensic Science Institutes (ENFSI) project titled “Steps Towards European Forensic Area (STEFA),” funded by the European Union. The software tool, based on popular statistical programming language R, is intended to provide a simple but powerful graphical user interface for forensic chemists to allow them to design and apply in practice the most common chemometric methods.

To determine the applicable methods, a literature survey was conducted as part of the project.[1] While not intended to be a comprehensive review, this survey was used to determine the most common use cases of chemometric methods in forensic chemistry literature, with a focus on illicit drugs. Based on these results, ChemoRe has been designed to be as intuitive as possible to apply to the typical workflow of forensic chemistry casework. This sets it apart from other similar software that also implement the same methods that tend to be more open-ended and require more statistical and computational expertise from their users.

ChemoRe acts as a bridge for its users to the powerful features of the statistical R-language through an interface, implemented with the Shiny framework that allows the user to design chemometric pipelines by a few clicks of the mouse.[2,3] This pipeline can be saved and validated within the software and subsequently converted to a ready method that can be applied to new case data. Additionally, the results obtained can be appropriately visualized to support interpretation and reporting of the results. This should make it attractive to forensic chemists who seek to make use of chemometric methods.

In this presentation, the ChemoRe software is introduced by presenting the relevant background on its development, including the results of the literature survey and main technical features. Furthermore, realistic example applications are introduced that show how chemometric methods can be applied to casework using ChemoRe.

Reference(s):

1. M. Bovens, B. Ahrens, I. Alberink, A. Nordgaard, T. Salonen, S. Huhtala. Chemometrics in forensic chemistry—Part I: Implications to the forensic workflow. *Forensic Science International*, Volume 301 (2019): 82-90.
2. R Core Team (2019). *R: A language and environment for statistical computing.* R Foundation for Statistical Computing, Vienna, Austria. https://www.R-project.org/.
3. Winston Chang, Joe Cheng, J.J. Allaire, Yihui Xie, and Jonathan McPherson (2019). *shiny: Web Application Framework for R.* https://CRAN.R-project.org/package=shiny.

Chemometrics, Forensic Chemistry, Statistical Methods

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