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Editor-in-Chief

Analytical Chemistry

Manuscript title: **Cost-efficient unsupervised sample selection for multivariate calibration**

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Other authors: Bart De Ketelaere, Ben Aernouts, Wouter Saeys

Dear Editor:

As part of our ongoing research on multivariate calibration model building, transferring and maintenance to contribute to higher efficiency and effectiveness in industrial applications, we produced this manuscript that addresses the topic of unsupervised sample selection in order to provide a generalized answer on how to approach this practice in real applications.

Motivated by the challenges revealed by industrial collaborators and the relevance of this topic as disseminated in major publications in the last decades, we tackled the problem from a broader theoretical perspective that allowed us to find answers that can be generalized to other applications. We hold a tight interest in knowing what the community would think of this perspective of the problem along with the practical solutions that we included in the manuscript.

Inspired by such a community, we aim to submit our research in the Analytical Chemistry Journal in order to obtain the fundamental feedback and dissemination for a topic that is of high interest within the academic and industrial chemometrics members.

As the topic is quite ample and the required experiments rendered multiple important results, we remained with the doubt of the appropriate length of the manuscript. According to a word-count estimation, the manuscript contains around 8000 to 9000 words. We put our best efforts to limit the content without compromising consistency and veracity. We consider the sections included in the manuscript to be highly relevant in order to understand the problem and the provided solutions.

The manuscript was prepared with the Latex template provided by ACS. The files for submission are the main manuscript with .tex extension, the figures in .png and .tiff formats and the generated PDF file using the mentioned template. We understand that the template for submission does not correspond to the template for publication. In regard to reproducibility and replicability of our work, a repository is already available containing all the methods and data used in the current work. This repository is currently private but with the possibility for publication according to the status of the current submission or the request by the Journal.

Motivated by the topic and the experts within the chemometrics field, we proposed this manuscript to be potentially revised by Tom Fearn, Tormod Naes, Asmund Rinnan, Oliver Tomic, Juan Antonio Fernandez Pierna and Michal Daszykowski.

We want to deeply thank you for your time to evaluate our submission.

Sincerely,

Valeria Fonseca Diaz

Bart De Ketelaere

Ben Aernouts

Wouter Saeys