Mapping Chemometrics with Chemometrics

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WHAT IS CHEMOMETRICS???

Chemometricians often face this question asked by students, laboratory analysts, chemists, and industry customers. Much effort is spent trying to come up with clear and concise answers, also considering the different levels of detail at which the question needs to be answered. Together with this question, we should probably also ask ourselves: "**where is Chemometrics**?".

Starting from the considerations proposed by José Amigo in 2021 [1], we believe that a discussion about the relationship between Chemometrics and the wide field of data science (does the latter includes the former, or vice versa?) should be started in our community.

This leads to a second important layer of the subject, which is about **how to "organize" and compare the methods and topics of Chemometrics**, according to their purpose(s) and uses, but also their characteristics.

*This could mean **describing Chemometrics with the tools of Chemometrics.***

But to do that we need you !!

*Help us building the **Map of Chemometrics!***

↓ an example of the form we will provide to you!

Please input the following methods:

- Principal Component Analysis (PCA)
- Projection Pursuit (PP)
- Procrustes analysis (PA)
- Independent Component Analysis (ICA)
- Multivariate Curve Resolution (MCR)
- Hierarchical clustering
- Partial Least Squares (PLS) regression
- Principal Component Regression (PCR)
- Multilinear Regression (MLR)
- Design of Experiments (DoE)
- OPLS

For each contribution, **candy will be provided**!

How

We would like to collect your opinions, here at CAC 2022 Conference, using the *Napping* technique [2].

1. ***Principle.***
   - **You are asked to** evaluate the similarities (or dissimilarities) among several chemometric methods**.**
   - **You have to do this according to your own criteria. You do not have to indicate the criteria. There is no good or bad answer.**
2. ***Procedure*.**
   - **We will provide the blank map on which you will have to position the methods, in such a way that two methods which are very close are almost identical, while if they end up distant, they seem different to you.**
   - **Again, this must be done according to your own criteria. Do not hesitate to express strongly the differences you perceive by using the most part of the sheet.**
   - **Please draw a full dot to clearly mark the position of each method.**
3. ***Data analysis.***
   - **Your napping results (the map you will draw) will be digitalized and converted into a set of Euclidean distances.**
   - **All "samples" collected from you will be organized as a numeric matrix that can be analyzed by Procrustes Multiple Factor Analysis [3], which provides, among the other outputs, a "consensus configuration", which looks like a map with all the evaluated objects on it.**

→ The consensus configuration will be our Map of Chemometrics!

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REFERENCES

[1] J.M. Amigo, *BrJAC*, **8**(32), (2021) 22-38
[2] J. Pagès, *FoodQual*, **16**(7), (2005) 642-649
[3] E. Morand, *FoodQual*, **17**(1-2), (2006) 36-42