



**HAL**  
open science

## **ChemHouse, a research and development centre for chemometrics**

Benoit B. Jaillais, Marion Brandolini-Bunlon, Jean-Claude Boulet, Gilles Chaix, Éric Latrille, Matthieu Lesnoff, Alexandre Mallet, Sílvia Mas Garcia, Maxime Metz, Virginie Rossard, et al.

► **To cite this version:**

Benoit B. Jaillais, Marion Brandolini-Bunlon, Jean-Claude Boulet, Gilles Chaix, Éric Latrille, et al.. ChemHouse, a research and development centre for chemometrics. Congrès Analytics 2022, Sep 2022, Nantes, France. 2022. hal-03910363

**HAL Id: hal-03910363**

**<https://hal.science/hal-03910363>**

Submitted on 29 Dec 2022

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# ChemHouse, a research and development centre for chemometrics

Benoît Jaillais<sup>1,2</sup>, Marion Brandolini-Bunlon<sup>2,3</sup>, Jean-Claude Boulet<sup>2,4</sup>, Gilles Chaix<sup>2,5,6</sup>, Eric Latrille<sup>2,7</sup>,  
 Matthieu Lesnoff<sup>2,8,9</sup>, Alexandre Mallet<sup>2,7,10</sup>, Silvia Mas Garcia<sup>2,11</sup>, Maxime Metz<sup>2,12</sup>,  
 Virginie Rossard<sup>2,7</sup>, Douglas N. Rutledge<sup>2,13</sup>, Rémi Servien<sup>2,7</sup>, Jean-Michel Roger<sup>2,11</sup>

1. ONIRIS, INRAE, StatSC, 44300 Nantes, France

2. ChemHouse Research Group, Montpellier, France

3. Université de Clermont Auvergne, INRAE, UNH, MetaboHub Clermont, Clermont-Ferrand, France

4. SPO, PROBE, INRAE, Montpellier SupAgro, University of Montpellier, F-34060, Montpellier, France

5. CIRAD, AGAP Institut, F-34398 Montpellier, France

6. AGAP Institut, Univ Montpellier, CIRAD, INRAE, Institut Agro, Montpellier, France

7. INRAE, Univ Montpellier, LBE, 102 Avenue des étangs, 11100 Narbonne, France

8. SELMET, Univ Montpellier, CIRAD, INRAE, Institut Agro, Montpellier, France

9. CIRAD, UMR SELMET, Montpellier, France

10. BioEnTech, F-11100 Narbonne, France

11. ITAP, INRAE, Institut Agro, University Montpellier, Montpellier, France

12. Pellenc Selective Technologies, 84120, Pertuis, France

13. National Wine and Grape Industry Centre, Charles Sturt University, Wagga Wagga, Australia

## ChemHouse, a research group

### Members

Around 50 experts, users, and students in chemometrics from public research institutes, R&D departments of industrial companies, NIR equipment suppliers, and scientific societies such as HelioSPIR

### Objective

To help the community and partners to overcome methodological barriers and difficulties in the use of chemometrics and to go beyond the current limits

## ChemProject



### ChemHouse (centre of expertise)

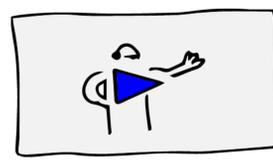
**Internal scientific seminars** (around 20 each year), on Near Infrared Spectroscopy data modeling, pre-processing of spectra, variable selection, variants of PLS modeling...

**Hosting of students and researchers** (for weeks to months, on average 9 months per year) to exchange on scientific subjects, and to improve their data processing skills.

**Organization of ponctual workshops and chemometrics events** such as ChemSchool (workshop in collaboration with the COST action Sensorfint) and HelioSPIR events.

**Initiation and collaboration on research projects**, to go deeper into data analysis by developing workflows, tools and algorithms:

- Participation in the setting up and implementation of national (Digitbio-MIMS) and international (Explore, AVITech) projects
- Co-author of scientific publications (more than 10 articles each year)



CheMOOCs

### CheMOOCs (Massive Open Online Course (MOOC))

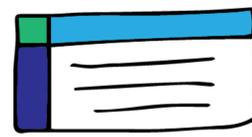
Annually followed by around 1500 people from over than 40 countries  
 28 training modules in 2 sessions: unsupervised and supervised methods.



ChemFlow

### ChemFlow (Galaxy instance)

Application of conventional and more advanced chemometrics  
 Interactive graphs  
 Able to upload of various data types



ChemData

### ChemData (database)

Datasets from the MOOC, from public projects of the ChemHouse group, or from external repositories.

**NEW**



ChemOmics

### ChemOmics (joint school)

Practical workshops and barcamp discussions between chemometricians and metabolomicians on methodological issues.

<https://chemproject.org/ChemHouse>

@list: [chemhouse@groupe.renater.fr](mailto:chemhouse@groupe.renater.fr)

@contact : [jean-michel.roger@inrae.fr](mailto:jean-michel.roger@inrae.fr)

Partenaires

