

ChemoSoft®

A new chemometric software for non-chemometricians

Christophe B.Y. CORDELLA

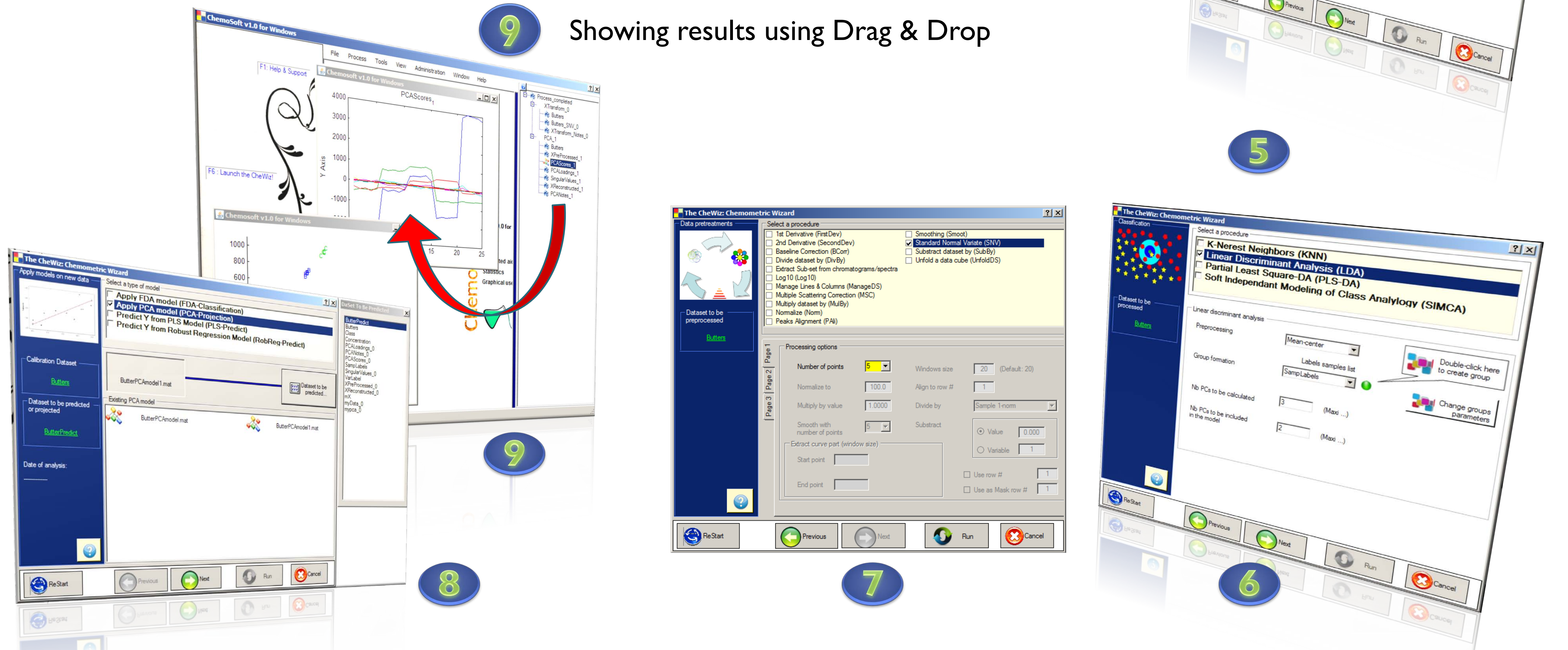
Analytical Chemistry Laboratory, UMR1145 GENIAL INRA/AgroParisTech
Equipe Ingénierie pour la Qualité des Aliments, 16 rue Claude Bernard – F-75005 PARIS
Christophe.cordella@agroparistech.fr



Visit our website and order a demo version
http://www.chimimetrie.fr/Chemosoft/crbst_2.html

ChemoSoft® v1.0 Interfaces

- 1 Main form (3 active tabs)
- 2 Chemometric Wizard (CheWiz), build your chemometric process
- 3 Selecting a target process to go to the appropriate tools (Exploration, classification, regression, preprocessing, visualization...)
- 4 Dedicated to data mining tools
- 5 Tools for linear regression
- 6 Classification tools
- 7 Data preprocessing (15 ≠)
- 8 Reuse of pre-recorded patterns
- 9 Showing results using Drag & Drop



ChemoSoft® is a fully graphical software dedicated to shaping and treatment of physicochemical data, spectroscopic and sensory. Designed for non-chemometricians or non-statisticians, it provides a statistical and chemometric tools together gradually, depending on the objectives dictated by the user (exploration, classification, regression, data preprocessing or simply display raw or preprocessed data).

EXPLORATORY

- ❖ Basic Statistics (BS)
- ❖ Principal Component Analysis (PCA)
- ❖ Hierarchical Cluster Analysis (HCA)
- ❖ K-Means (KM)

CLASSIFICATION

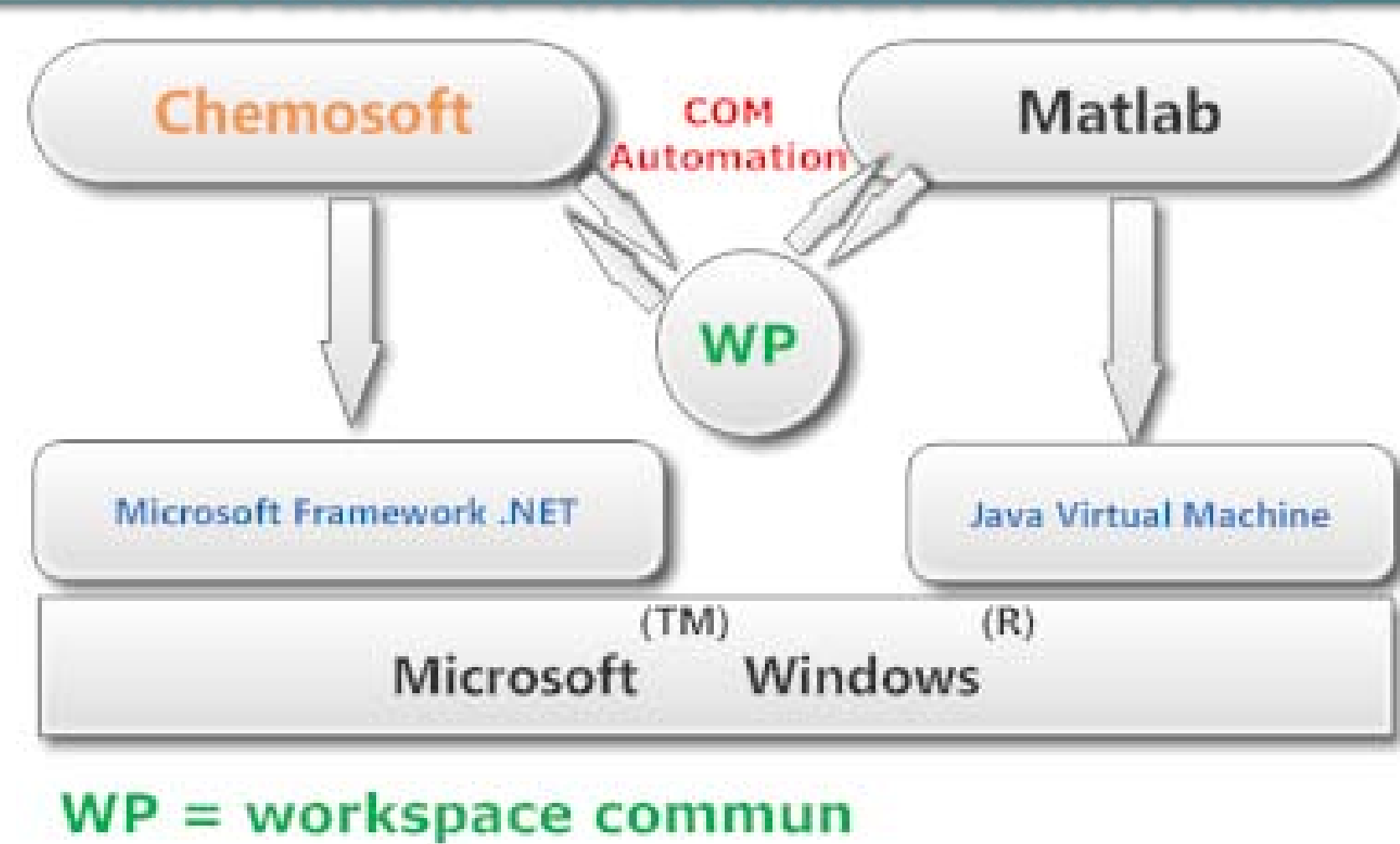
- ❖ K Nearest Neighbors (KNN)
- ❖ Linear Discriminant Analysis (LDA)
- ❖ PLS-Discriminant Analysis (PLS-DA)
- ❖ SIMCA

LINEAR REGRESSION

- ❖ Partial Least Squares (PLS-I & PLS-2)
- ❖ Principal Component Regression (PCR)
- ❖ Robust Regression (RobReg)

Available
Under development

INTERFAÇAGE AVEC MATLAB



WP = workspace commun

The workspace of **ChemoSoft** is linked to that of **Matlab**. Matlab runs a special memory area called "**Workspace**" in which all objects (matrices , vectors, cells , structures, string ...) are stored in a session .

ChemoSoft is sharing this memory area with Matlab via a specific communication called "**COM Automation**". To do this, Matlab must operate as a **COM server**. COM is used in applications such as the products of Microsoft Office family. For example, "OLE COM" technology allows Word documents to dynamically link to data in Excel spreadsheets and "**COM Automation**" allows users to create scripts in their applications to perform repetitive tasks or control of an application by another .

Finally, you use Matlab objects without needing to know its syntax or its operations, and you enjoy its computing power.

**** Christophe B.Y. Cordella, Dominique Bertrand. SAISIR: a new general chemometric toolbox. Trends in Analytical Chemistry, 2014, 54, 75-82. The article contains the link to freely download the toolbox.**

OS : Win XP Pro, SP2, SP3
Win 7, 2000 SP1
Matlab : v7.5 + Statistical toolbox

Environnement s : Microsoft Visual Studio 2010
Matlab v7.5
Langage : VB.NET (Visual Basic objets)