

Chemometrics in Forensic Science: Approaches and Applications

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Table S1: Comparison of common commercial and open source software packages for chemometric data analysis.

Software and OS Compatibility	Licensing Options	Range of Functionalities	Indicative Pricing (1 Year Single-User License) Estimates given in \$USD
MATLAB (Mathworks, USA) For Windows, macOS, Linux	Annual or perpetual	Most chemometric functionalities require a separate Toolbox add-on. The Statistics and Machine Learning Toolbox (Mathworks) offers a broad range of pattern recognition, regression and experimental design methods. The Deep Learning Toolbox (Mathworks) or PLS Toolbox (Eigenvector Research) enable expanded pattern recognition, regression and data pre-processing options	MATLAB: \$815 Mathworks Toolboxes: \$405 - \$470 PLS Toolbox: \$2095
The Unscrambler X (Camo Analytics, Norway) For Windows only	Single- and multi-user plans (minimum 6 months), term or perpetual licensing.	Base software offers a broad range of data pre-processing, pattern recognition and regression methods. Versions 10.4 onwards are bundled with Design-Expert (Stat-Ease, USA), enabling experimental design	\$1,000
The Unscrambler HSI (Camo Analytics, Norway) For Windows only	Single-user annual license	Basic pattern recognition, regression and experimental design methods for hyperspectral image analysis	\$1,200
R (R Core Team) For Windows, macOS, Linux	Open source	Effectively unlimited; new functionalities can be coded and shared	Open source
IBM SPSS Statistics (IBM Corporation, USA) For Windows, macOS	Single- and multi-user plans (monthly or annual), term or perpetual licensing.	Basic pattern recognition and regression	\$1,020
Minitab (Minitab LLC, USA) For Windows, macOS	Single- and multi-user plans (minimum 6 months) or perpetual licensing.	Basic pattern recognition and regression, as well as a broad range of experimental design options	\$1,230
XLStat (Addinsoft, Paris) For Windows, macOS	Single- and multi-user plans (minimum 12 months).	Basic version offers basic pattern recognition and regression analysis. XLSTAT Basic Plus enables expanded pattern recognition and regression, while XLSTAT Premium enables experimental design	XLSTAT Basic: \$295 XLSTAT Basic Plus: \$495 XLSTAT Premium: \$1495
SIMCA (MKS/Umetrics, Sweden) For Windows only	Single-user license with annual maintenance support fee.	Basic pattern recognition, regression and design of experiment methods scriptable using Python	\$1,720