

# A chemometrics toolbox



## Pirouette

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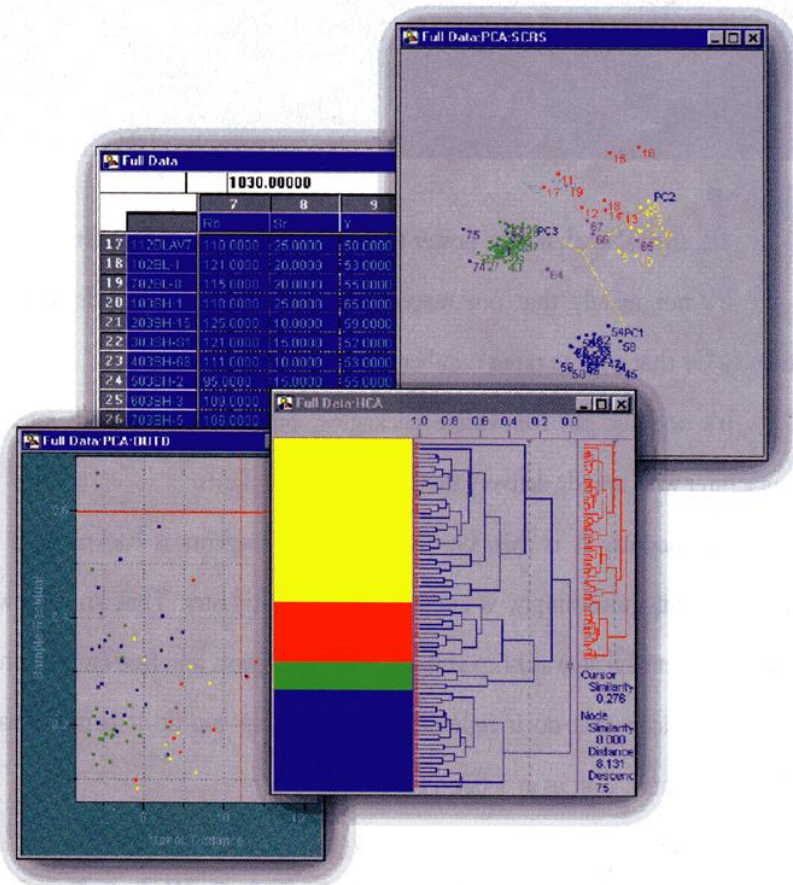
*Pirouette* is a versatile chemometrics toolbox for the Windows 95 and Windows NT operating systems. I evaluated it using two computer systems: a Pentium Pro 200-MHz machine with 64 MB of RAM running Windows NT 4.0 and a 100-MHz Pentium notebook computer with 16 MB of RAM running Windows 95. In terms of the look and feel, *Pirouette* uses the common Windows 3.1 dialog boxes for opening and saving files. This method can present a problem for networked computers because nodes in the network neighborhood are not recognized. Although *Pirouette* does not support Object Linking and Embedding (OLE), it does support cutting and pasting of tables as unformatted text and figures as device-independent bitmaps (DIBs). I evaluated *Pirouette* with Microsoft Word 7.0 and Excel 7.0 for transferring data and figures between applications.

*Pirouette* is easy to learn and use. Most of the basic chemometric methods, such as hierarchical cluster analysis (HCA), principal component analysis (PCA), K-nearest neighbors (KNN), Soft Independent Modeling for Class Anal-

gies (SIMCA), partial least squares (PLS), and principal component regression (PCR), are readily available. These individual methods are all interfaced in an object-oriented fashion, which is the strength of *Pirouette*. For example, using HCA, the user can define class assignments for objects, and *Pirouette* automatically assigns colors for each class; these same colors will be mapped onto objects in other charts generated from separate chemometric analyses. *Pirouette* is miss-

ing a linear discriminant analysis (LDA) method, which is a standard classification method.

The object manager follows the same type of design with folders as the file manager in Windows uses for files, which allows the user to organize results and graphs of numerous methods. However, one cannot move to a chart by double clicking in the object manager, and multiple graphs in the same user-defined window cannot be manipulated together (e.g.,



*Pirouette* includes all of the basic chemometric methods, including HCA.

