

## MINITAB Release 14

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MINITAB Release 14 is the latest version of the popular statistical and analysis and process management program for Windows. This new version offers improved usability and graphics over previous versions, plus an expanded range of statistical functions.

On opening the package I was pleased to see that, unusually for software nowadays, a paper manual was included. Although “Meet MINITAB” is more of a tutorial than a reference guide, I found the investment of a couple of hours to run through the nine short examples informative and worthwhile.

After completing the tutorials, I decided to take a shot at doing something substantial with some real chemical data. For my first experiment, I chose to simulate a simple QSAR experiment by using a 42 674 subset of the NCI data set for which AIDS activity classifications had been generated (three classifications—Active, Moderate, or Inactive). For each compound, I generated 1052-bit 2D structural fingerprint data, resulting in a file of 1052 descriptors plus a name and activity classification for each compound. This is well within Minitab’s limits (4000 columns).

Trying to open the file was painful—it took literally about 30 minutes of the hourglass cursor before the program reported that it had run out of memory (the machine I was using had a reasonable 640MB). I was able to load a shortened version of the file with only 5000 rows but soon found that navigating to any menu that involved selection of descriptors resulted in the dreaded hourglass and a wait long enough for me to close the program down and start again.

After concluding that MINITAB is not really up to handling this number of descriptors, I abandoned plans to use fingerprint data and instead read in a file containing 10 property descriptors (CLOGP, HBA count, etc.) for each of the 340 structures. This proved a much more successful experiment. It was very easy to produce some basic statistical graphs of good quality (histogram distributions of values, individual value plots, regression analysis, and so on); the

graphical summary is nice. The graphs are aesthetically pleasing, better than previous versions of MINITAB and far better than the default graphs in Microsoft Excel. The program has a good range of statistics available ranging from basic to advanced, including extensive experimental design and quality assessment. Of particular note for those in QSAR and related fields is the addition in this version of Partial Least Squares (PLS) as part of the regression analysis package.

Statistical Software is not exactly renowned for clarity or ease of use, and there are certainly some usability improvements that could be made to MINITAB. However, I was generally very impressed with the efforts that have been made to make the program straightforward to use and to tame its complexity (including a reasonable help system), and features such as the layout and project managers make keeping track of many windows easier. Menus are laid out in a fairly logical fashion, although finding the right place to set particular options or parameter settings can be something of an adventure. The quality of the graphics is noticeably improved over previous versions.

Overall, I would heartily recommend MINITAB for those wishing to do basic and advanced statistics on data containing tens or maybe a hundred or so descriptors, and with no requirement to include 2D chemical structure visualizations (MINITAB has no functionality specific to the chemical community). The range of functionality and program usability is good: a novice user could probably be producing useful statistics in a couple of hours. For existing MINITAB users, the addition of PLS plus numerous graphics and ease-of-use improvements makes an upgrade at least worth considering.

MINITAB costs \$1195 for a single copy (with discounts for multiple copies) or \$395 for an upgrade. More information is available at [www.minitab.com](http://www.minitab.com) or by calling (800) 448-3555 inside the United States.

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