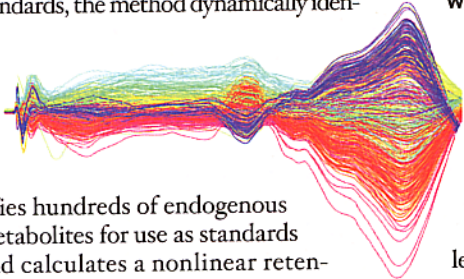


# DIGITAL BRIEFS

NEW SOFTWARE AND WEBSITES FOR THE CHEMICAL ENTERPRISE

## Software

**XCMS** is a new open-source program for accurate metabolite profiling. It is an LC/MS-based data analysis approach that incorporates novel nonlinear retention time alignment, matched filtration, peak detection, and peak matching. Without using internal standards, the method dynamically iden-



tifies hundreds of endogenous metabolites for use as standards and calculates a nonlinear retention time correction profile for each sample. Following retention time correction, the relative metabolite ion intensities are directly compared to identify changes in specific endogenous metabolites, such as potential biomarkers. XCMS is freely available for Windows or Macintosh under an open-source license at <http://metlin.scripps.edu/download>.

**Un-Scan-It Gel 6.1** software turns a scanner into a high-speed densitometer and allows users to automatically analyze gel images at

full scanner resolution. It works with any scanner, digital camera, or other image input device to digitize electrophoresis gels. In addition to the gel analysis features, the software also contains (x,y) digitizing and graphing features. The digitized gel and (x,y) data can be exported into most other software programs. The software is available for Windows and Macintosh. **Silk Scientific**, [www.silkscientific.com](http://www.silkscientific.com)

**TT900 S25** is an advanced image alignment application used to generate high-quality 2-D image analysis results. The software corrects the various gel inconsistencies that occur when running and imaging 2-D electrophoresis gels. Once aligned to a very detailed level, images can be exported for traditional gel analysis. **Nonlinear Dynamics**, [www.nonlinear.com](http://www.nonlinear.com)

**The Sentient Suite** allows a user to assemble, view, analyze, annotate, and search disparate information in a common environment. The disparate data can be numeric values, images, spreadsheets, Web content, public or private databases, or information from applications such as structures and reactions in ISIS, analytical results (GC/MS, IR, and others), and Excel spreadsheets. Sentient runs on Windows in a server model for