ProteinChip® Data Manager Software

Powerful Software for Collecting, Analyzing, and Organizing Data for Biomarker Discovery

The search for clinical biomarkers involves the analysis of large numbers of patient samples, and when combined with the ProteinChip SELDI system's high-sensitivity, high-throughput capabilities, the result is an enormous amount of data. The ability of clinical researchers to mine this data and uncover possible biomarkers is directly dependent on the quality of the software tools available. ProteinChip data manager software is designed to provide a biomarker discovery toolset that drastically reduces the time required for data analysis. The software encompasses all aspects of the process, from instrument control through creation of a list of candidate biomarkers of statistical significance.

- Streamlined analysis of protein profiling data
- Intuitive graphical interface
- Organization, display, and processing of thousands of spectra
- Univariate and multivariate statistics for selecting candidate biomarkers
- New Desktop Edition for project collaboration and remote data analysis

For more information about ProteinChip products, visit us on the Web at **www.bio-rad.com/proteinchip/**.
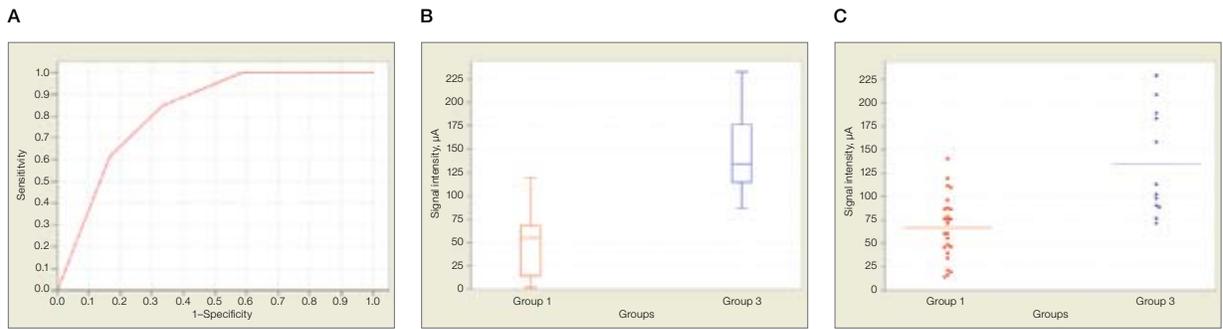
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Fig 1. Receiver-operating characteristic (ROC) plot (A) and corresponding box-and-whisker (B) and mass scatter (C) plots visually display protein expression levels across groups.

Integrated Instrument Control

For most samples, the simplified instrument control interface of ProteinChip data manager software takes the large number of settings normally required to acquire data and reduces them to the most important input commands. For applications requiring more flexibility, the software's advanced protocols are used to fine-tune parameters.

Complete Spectrum Processing and Biomarker Analysis Toolset

Biomarker discovery involves the search for proteins whose expression levels differ from one sample group to another. ProteinChip data manager software includes the tools necessary to uncover biomarkers hidden in the large amounts of information produced by the ProteinChip SELDI system. The software includes spectrum processing algorithms to reduce spectrum noise, align spectral masses, and normalize peak intensities.

The peak clustering feature of ProteinChip data manager software groups peaks of similar molecular weight from across sample groups of spectra and visually displays differences in expression levels. Built-in *P* values and ROC curves are used to report statistical relevance for individual markers (Figure 1).

The software includes additional statistical tools, such as hierarchical clustering and principal component analysis (PCA) (Figure 2), for analyzing the relationship between samples. Export formats are compatible with other tools.
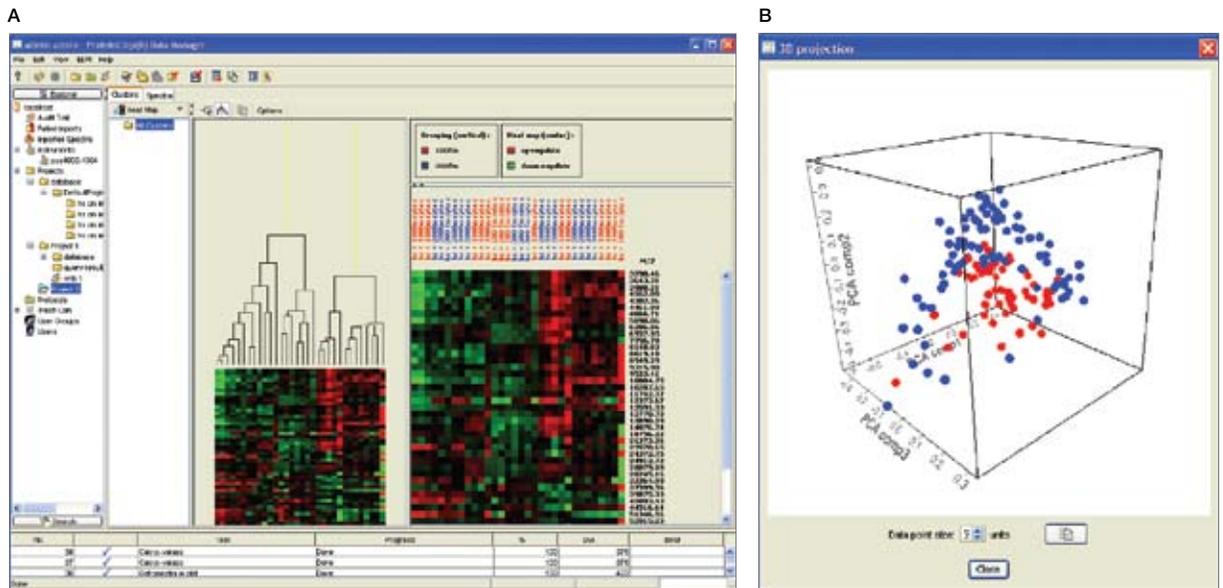

Fig 2. Examples of multivariate analyses. A, a heat map generated by hierarchical clustering and **B**, a PCA plot allow exploration of the relationship of expression levels between samples.

Sample Tracking

ProteinChip data manager software provides an intuitive, graphical user interface for fast, easy input of sample properties and acquisition parameters using the Virtual Notebook (Figure 3). The Virtual Notebook allows the user to enter comprehensive information on sample processing conditions associated with each spot on the arrays. During unattended acquisition, the ProteinChip SELDI reader communicates with the data manager server to transfer the sample property and acquisition information from the Virtual Notebook for up to 1,344 unique samples. Spectra are then exported to the data manager, fully annotated and ready for further downstream analysis.
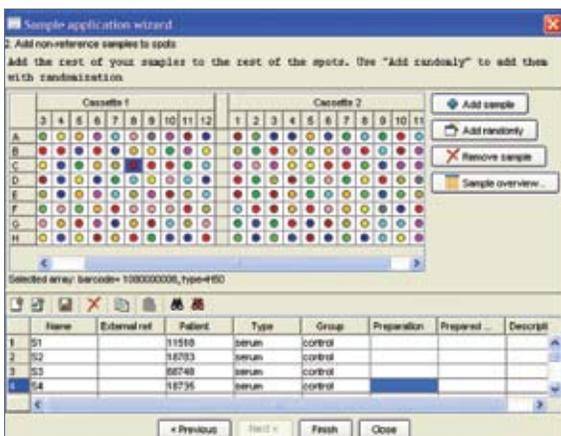

Fig. 3. Virtual Notebook assists with array layout and annotating sample information.

System Operational Qualification

As with any scientific study, the calibration of the platform must be monitored closely at regular intervals to ensure maximum reproducibility. The software works in conjunction with ProteinChip operational qualification (OQ) kits to provide calibration results for the ProteinChip SELDI reader from a single mouse click. The software automates the application of necessary processing parameters, labels the required peaks, and generates a PDF report of the results (Figure 4).

Fig 4. OQ report rapidly qualifies instrument performance.

Biomarker Analysis Guide

The details of the biomarker analysis workflow are explained further in the guide entitled Biomarker Discovery Using SELDI Technology — A Guide to Data Processing and Analysis Using ProteinChip® Data Manager Software, available on the web at **http://www.bio-rad.com/ad/biomarkerguide/**.

The guide includes the following topics:

- Description of the data analysis steps, beginning with data organization and proceeding through statistical analysis of peak clusters
- Detailed information about many of the software's analysis features
- Settings recommendations for different data sets
- Appendices containing a glossary of software terms and a workflow summary

Software Configurations

The new ProteinChip data manager software, Desktop Edition provides researchers with full-featured software that can be used remotely, making it useful for collaborative projects and off-site data analysis. For users of older systems, it serves as a great way to update to the latest biomarker analysis algorithms. The Enterprise and Personal Editions of software are shipped with the ProteinChip SELDI Enterprise and Personal readers, respectively.
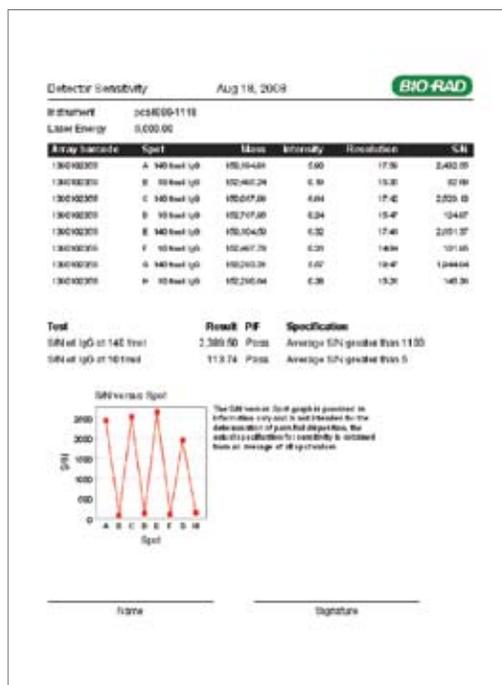
Software Feature	Enterprise Edition	Personal Edition	Desktop Edition
Protein profiling data analysis toolset (including P values, ROC curves, and trend plots)	Yes	Yes	Yes
ProteinChip SELDI reader control	Yes	Yes	No
OQ kit compatibility	Yes	Yes	Yes
Sample tracking with Virtual Notebook	Yes	No	No
Audit trail	Yes	No	No
Server/client	Yes	Yes	No
Offline data analysis	No	No	Yes

Enhancing the Biomarker Research Process — Version 4

Version 4 of ProteinChip data manager software introduces a number of new features that enhance clinical research workflows by further streamlining data processing and analysis steps, enabling new data visualizations, and creating a new time point analysis plot.

Analysis Wizard

Previous versions of ProteinChip data manager software had separate dialogs for data processing and analysis, and required the manual input of parameters for each new set of data. In version 4, data processing, normalization, and clustering have been brought together into a single, new Analysis Wizard, lessening the amount of clicking back and forth. More importantly, the parameters set in the Analysis Wizard can now be saved and rapidly applied to other data sets.

Spectrum Overlay Plots

Version 4 introduces spectrum overlay plots to the software (Figure 5). In combination with the ability to assign colors to spectra, researchers now have a powerful new plot display for visualizing protein expression changes between sample groups. Overlay plots can even be rotated to produce landscape spectrum views.
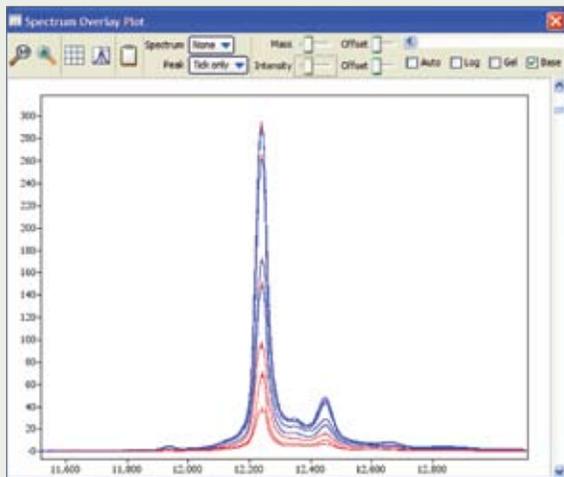

Fig. 5. Spectrum overlay plot for quick spectrum comparisons.

Trend Plots

Trend plots give researchers the ability to track clustered data along an additional time point axis by plotting the expression level of a cluster as a function of multiple readings. With trend plots, researchers can now visualize the expression level changes of potential biomarkers over the course of multiple patient samplings or varying dosages (Figure 6).
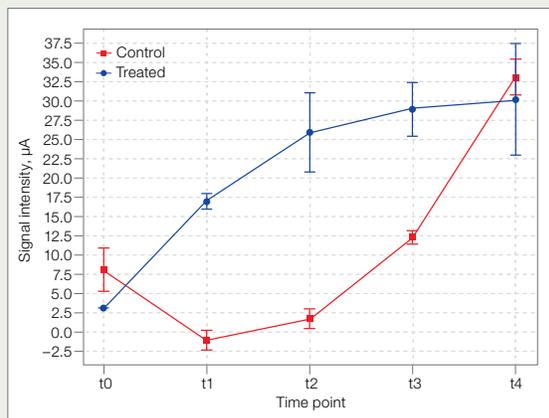

Fig. 6. Trend plot tracks expression over time between sample groups.

New Look and Feel

The user interface has been redesigned to accommodate new spectrum navigation and plotting features. Graphs have been updated to achieve presentation-ready quality. Spectrum navigation and zooming have been improved to further enhance biomarker analysis.

Ordering Information

Catalog #	Description
SW3-040010	**ProteinChip Data Manager Software 4, Personal Edition**, includes 1-user network license
SW3-040030	**ProteinChip Data Manager Software 4, Enterprise Edition**, includes 5-user network license
SW3-040050	**ProteinChip Data Manager Software 4, Desktop Edition**, includes 1-user network license, no instrument control
SW3-020050	**ProteinChip Data Manager Software 4, Add 1 User to Network License**
SW3-060010	**ProteinChip Data Manager Software 4 Upgrade**, version 3.x to 4 upgrade
SW3-060030	**ProteinChip Data Manager Software, Desktop Edition and Server Upgrade Bundle**

The SELDI process is covered by U.S. patents 5,719,060; 6,225,047; 6,579,719; and 6,818,411 and other issued patents and pending applications in the U.S. and other jurisdictions.