

Release Notes for ProteinChip® Software

Release 3.0

IMPORTANT NOTE

This release of the software uses a database and files to store experiments and data. Do not delete, rename or move files or folders under the database folder, or your data will be corrupted or lost! See the applicable sections of the manual for details on how to import and export data into and out of the database, and how to backup and move databases.

This version of the software can co-exist on a computer with Release 2.1. Files from earlier releases can be read by this version of the software, but please remember that files exported from this version can only be read by Release 3.0 software or later releases.

If you install this version on a computer with a previous version of 3.0 (alpha 1, alpha 2, or beta 1, or beta 2) installed, uninstall the previous version before installing the release. To uninstall the previous version, use add/remove programs under the control panel and select CIPHERGEN ProteinChip 3.0. Select Remove from the options dialog, which will remove the previous version of the program. Uninstalling the software will not erase your data files or database.

If you encounter a problem, please read the known issues at the end of this note, and if the problem hasn't already been documented, write a problem report. The report should include as many of the details as you can give us about the problem, the version number of the software (found in the about box), and whether you can reproduce the problem. If the problem involves an experiment or spectrum file, please attach it to the report. Please send problem reports to: software@ciphergen.com

Summaries of the issues that have been fixed since the first alpha are listed at the end of this note.

SIGNIFICANT ENHANCEMENTS SINCE 3.0 BETA RC1

- The PBS II Plus instrument can be chosen from the Instrument Selection dialog.
- Manual acquisition speed has been lowered from 10 shots per second down to 4 shots per second.

SIGNIFICANT ENHANCEMENTS SINCE 3.0 BETA 2

- Several new capabilities have been added to the instrument control software. These capabilities are inactive by default, and can be accessed and enabled from the Instrument Configuration dialogs Options... button. The new capabilities include:
 - The Instrument Source can be automatically conditioned after 7 days of non-operation.
 - The instrument serial number and name can be entered and will be stored with the spectrum data.
 - The laser can be automatically normalized to adapt for the loss of laser energy over time.
 - The Laser Neutral Density Filter can be extensively tested for proper operation at instrument initialization.

- Instrument usage data including the number of sample exchange cycles, and the number of laser shots, can now be recorded. This information can be used to help determine routine instrument service needs.
- Opening/creating a database is now via a Database Connection Wizard.
- Users can log off. This is accessed from the File Menu by selecting the Log Off menu item.
- Biomarker Wizard can generate Biomarker Patterns file without estimated peaks and exports blanks in their place.
- Creating new users initializes settings based on factory defaults, not the Guest user.

SIGNIFICANT ENHANCEMENTS SINCE 3.0 BETA 1

- The speed of data acquisition for an experiment has been increased by 40%.
- Sizing of the experiment window has been changed back to its original behavior, where the size can only be changed through the Presentation Protocols.
- Newly created users will have available All-in-1 Peptide and Protein calibration protocols added to the protocol list. In addition, all new users' settings will be based on a default user template.
- A batch import tool has been included which can import and save multiple experiments to the database automatically. This option can be found under File | Import | Batch...

SIGNIFICANT ENHANCEMENTS SINCE 3.0 ALPHA 2

- A sorting function is available for sorting experiments. It's accessed by selecting Experiment | Sort Item...
- You can select multiple experiments for import in the import file dialog. Hold the shift or control key to select multiple files.
- The current list of peptide and protein standards has been updated in the program. In order to see the new standards in the calibrants list however, you must create a new user and select based on 'Nobody'.
- There is a database integrity check feature that will tell the user if there are files missing or broken links in the database. This is accessible via Options | Run database check in the main menu.
- The dialogs used for saving spectra and experiments and creating projects have been improved to show existing ones. The user doesn't have to "guess" at a unique name.
- The noise window can now be linked with the filter setting (Analysis Protocols/Noise). The default remains at least 21 data points but you can now select a multiple of the filter window width instead. This setting is now saved with the spectra.

SIGNIFICANT ENHANCEMENTS SINCE 3.0 ALPHA 1

- The installation now works on NT 4.0 and PC's that don't have Microsoft Office installed.
- The login dialog is now separate from the exchange dialog.
- The process of creating a new database and browsing for an existing database has been improved. You can now create a new directory from the Initialize Database Connection dialog.
- The user interface of the Biomarker Wizard has been enhanced to make it easier to use for both automatic and semi-manual peak detection.
- The Biomarker Wizard Plot can be copied to the clipboard.
- This version enables data collection.
- The restriction on opening files from different projects at the same time has been removed.
- Several of the larger dialogs such as the sample properties, are now resizable.

- A 'backdoor' password has been added in order to recover data where the password has been forgotten. Call us if you need it.
- The selected spectra in an experiment are copied to the clipboard, rather than all of them.

NEW FEATURES IN RELEASE 3.0

Database

Many of the enhancements to this version are enabled by using a database to store important information about the data. The database allows the software to build new experiments from existing spectra, and to sort and manage the spectra properties. These properties include the sample information associated with each spectra along with all of the ProteinChip® protocol conditions such as the type of ProteinChip array, the wash conditions and the data collection parameters. This arrangement makes it easy to construct experiments for the conditions that you wish to analyze, and will allow much greater flexibility with data management in future versions.

Biomarker Wizard

The Biomarker Wizard has been significantly enhanced. The important changes include:

- The output of Biomarker Wizard is now in a splitter window. The mass range of the plot tracks the experiment.
- A 'Box and Whisker' plot is available to summarize complex biomarker patterns.
- The clustering now allows the use of manual peaks. This allows you to define the peaks of interest in a few spectra and then allow Biomarker Wizard to find or estimate the peaks for the remaining spectra.
- Peak clusters can be saved and reloaded to another experiment. This allows you to compare the same markers across multiple experiments.
- Biomarker Wizard can export data in a format compatible with the Biomarker Patterns Software.

Normalization

A new option in the normalization dialog allows normalizing to total ion current. This method generally reduces the average variation of spectra across an experiment, and is the recommended default for expression profiling.

Signal Enhancement

A new option in the Filtering dialog enables a variable gain setting for high mass plus an additional filtering step. The combination improves the signal to noise ratio of high mass peaks. To use the feature, check the 'Signal Enhance' checkbox on the Filtering tab of the Analysis Protocol Properties.

Mass Calibration Equation

The form of the mass calibration has been changed from a cubic to a quadratic fit to allow calculating the high order coefficients with fewer calibration peaks. The mass accuracy of internal calibrations can be greatly improved over the linear defaults that the previous algorithm used.

Another significant improvement to the mass calibration is how calibrations are adjusted when using a single point calibration. Previous versions of the software required at least two points for an accurate mass calibration whereas this version will generate better calibrations with even a single internal standard.

Calibration Protocols

Calibration Protocols automate the process of mass calibration. The protocols contain a list of mass calibrants and rules that allow the software to identify the calibration peaks and generate a new mass calibration. This makes utilizing a mass standard such as the all in one peptide mix much easier. In addition, the calibration protocols can be applied to multiple spectra in an experiment, allowing you to align the mass of common peaks in a series of spectra from a protein profiling or other SELDI experiment.

Calibration Equations

The software now allows saving a calibration equation from a spectrum and applying calibration equations to one or more spectra.

KNOWN PROBLEMS IN RELEASE 3.0

The following issues have been deferred to the next release:

[Problem ID: 1381] Performing mass normalization can result in a software crash when multiple instances of the same mass are added.

[Problem ID: 1584] Launching software by double clicking an xpt file results in a Windows error message. The application still starts up ok and loads the desired xpt file.

[Problem ID: 1585] xpt files have the wrong icon

[Problem ID: 1583] No error when source or detector control boards unplugged during data acquisition

KNOWN PROBLEMS IN RELEASE 3.0 BETA 2

[Problem ID: 1291] Can't import CSV files. (Note: This may be deferred until the next release, and more functionality can be added to import.)

[Problem ID: 1351] The Biomarker Plots don't update when intensity or mass values change.

[Problem ID: 1472] The Biomarker Patterns file is incomplete when clusters are incomplete. Only spectra with complete membership in all clusters get reported in this file. This problem arises when adding estimated peaks is turned off in BMW.

[Problem ID: 1473] Sample group statistics may be incorrect when clusters are incomplete. This problem arises when adding estimated peaks is turned off in BMW.

Note: A warning will appear if the sample group statistics is selected after having estimated peaks turned off.

SUMMARY OF PROBLEMS RESOLVED SINCE ALPHA 1

[Problem ID: 1290] Non-standard characters disable ability to save experiments. Characters, such as an apostrophe, cause an assert in debug mode, and ignoring the asserts leads to an "error in creating new experiment" error message box.

[Problem ID: 1315] Loading clusters from a file seems to have some numerical errors. Some cluster masses end up being $-6.27743856220419E+66$ (this is apparent when you look at the statistics report generated from the experiment in which you loaded the clusters).

[Problem ID: 1322] If there isn't a database selected at program startup, a prompt will ask if you want to create a new database or press No to browse and select an existing database. **If you select no and don't have a database, the program won't allow you to exit.** If you get into this unfortunate loop, use the task manager to exit the program.

[Problem ID: 1323] Changing any of the options on the Display tab of the presentation protocol doesn't work if the spectra are in an Experiment. It does work if the spectra are displayed individually.

[Problem ID: 1330] Alpha 1 won't install reliably on NT 4.0.

[Problem ID: 1342] Copy only selected spectra to the clipboard.

[Problem ID: 1365] Rescale the signal enhancer to a 'normal' 0-100 range.

[Problem ID: 1383] Add the peaks used for mass normalization to the normalization summary dialog.

SUMMARY OF PROBLEMS RESOLVED SINCE ALPHA 2

[Problem ID: 1221] Linking noise window with filter setting. The fix is for evaluation only and does not get saved with the spectra in the beta release.

[Problem ID: 1315] Cannot edit samples through Open | Samples... dialog if any sample names were left blank. This is mainly an issue with imported data files with blank sample names.

[Problem ID: 1321] Switching to Gel view does not resize the gel to the specified gel height automatically. If any of the heights in the Presentation Protocols are changed, however, the gel resizes properly.

[Problem ID: 1354] Editing a chip doesn't get stored to the database.

[Problem ID: 1398] If multiple spectra are highlighted for deletion, either by the ctrl-click or shift-click method, the user is prompted to confirm each deletion individually.

[Problem ID: 1409] Gel view does not resize upon applying.

[Problem ID: 1425] An error message appears when using the index function in the help screen. This doesn't appear to affect the search.

[Problem ID: 1431] Peaks crashes when an experiment with a synthetic spectra is exported to Excel.

[Problem ID: 1432]
Software crashes after clearing all peaks immediately after running Biomarker Wizard.

[Problem ID: 1434] Handle use of apostrophes in strings that get stored in db. SQL statements use single quotes around strings and apostrophes must be preceded by another apostrophe in these SQL statements.

[Problem ID: 1449] Software crashes when opening sample properties of experiment containing a synthetic spectrum

SUMMARY OF PROBLEMS RESOLVED SINCE BETA 1

[Problem ID: 1399] Occasionally the created Biomarker Plot makes the experiment windows too large for the screen.

[Problem ID: 1407] The sample properties dialog displays the hard shot laser intensity instead of specified laser intensity.

[Problem ID: 1454] Cannot left and right arrow scroll when the BMW view has focus.

[Problem ID: 1462] Calibration protocol crashes when applied to a synthetic spectrum.

[Problem ID: 1471] The program crashes if you run BMW without adding estimated peaks and some sample groups are not represented in one or more clusters. This happens when trying to generate sample group statistics.

[Problem ID: 1474] The BMW menu isn't enabled when the BMW plot is selected.

[Problem ID: 1476] Copying a spectrum causes it to lose its mass normalization.

SUMMARY OF PROBLEMS RESOLVED SINCE BETA 2

[Problem ID: 1532] Normalization of spectra of different mass ranges defaults to setting the range to the shortest spectrum.

[Problem ID: 1534] Peak dialog box not functioning properly.

[Problem ID: 1558] Copying a spectrum from the data average window does not copy the acquisition range.

[Problem ID: 1565] Centroiding does not work on "uninitialized" spectra that have not been rendered on the screen yet.

[Problem ID: 1571] Peaks crashes when selecting the calibration equations menu after deleting spectra.

[Problem ID: 1574] Column heading sort is broken in the Open/Delete Experiment and Open Project dialogs.

[Problem ID: 1582] Add code to support the digitizer watchdog timer so failures of the digitizer will not lock up the system.

SUMMARY OF PROBLEMS RESOLVED SINCE BETA RC1

[Problem ID: 1606] Fixed a problem that had led to a slowdown in acquisition speed.