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Installation Notes for Scaffold Q+ 3.3.2

In this version of Scaffold Q+ we have significantly changed the method of normalization for datasets containing two or more experiments. Previously, an attempt was made to normalize between experiments, and all ratios were calculated against the first reference channel. We found that this inter-experimental normalization was not effective and was producing invalid statistical results in some cases. In this version, we have done away with the normalization between experiments, and we now calculate the ratios for each experiment individually. As a result, Scaffold Q+ now supports within-subject experimental designs.

Installation Notes for Scaffold 3.3

Beginning with version 3.3.1, Scaffold should exhibit markedly improved performance in many areas. We have made changes that should significantly speed up merging of data files, renaming and reorganizing of biosamples, changing views, especially when opening the statistics view, and loading large Mascot DAT files, as well as indexing large databases.

We have also added an additional option to the Advanced Preferences menu which should be helpful to Proteome Discoverer users searching with Sequest. This new option, which is now the default selection, is called auto-detect. If this option is selected, Scaffold will scan the .msf file for spectra which have only one reported match. This should be a relatively rare occurrence, and if the percentage of such spectra is high, it is probably a result of filtering of peptide results within Proteome Discoverer. Such filtering makes it impossible to calculate an accurate delta Cn value and interferes with Scaffold's prophet algorithms, so if auto-detect determines that fewer than 90% of the spectra have proper delta Cn values, it uses the Xcorr only option in loading the data. Otherwise, the usual discriminant function is used. If the user selects a different option through the Advanced Preferences menu, that choice will be respected.

For any users who did not install Scaffold 3.2.0, you should be aware that beginning with that version, we made significant changes in how the program is installed on your computer. Now the parameters and logs will be stored separately for each user in his/her own file space. This will eliminate conflicts with Windows' User Account Control system, and eliminate many permissions problems encountered in Linux as well. It will also allow different users sharing the same computer to customize Scaffold in their own ways. For example, each user can have his/her own memory settings, collection of fasta databases, etc.

When Scaffold 3.2.0 or higher is first installed, it will check the directory into which it is being written, and if there are already settings in the parameters folder, it will copy them to the file space of the user who is installing the program. Hence, when the new version is run for the first time, it will assume the settings of the previous version. Any changes that the user makes after installation, however, will apply only when Scaffold is run from his/her account. If Scaffold 3.2.0 or higher has been installed by an

administrator, other users may run Scaffold, and their parameters will also be initialized based on the settings from the old version.

The **parameters** and **logs** folders will be written to the following directories:

Windows:

C:\Users\username\AppData\Roaming\Proteome Software\Scaffold

Linux:

/home/<username>/ .config

Mac:

/Users/<username>/Library/Application Support/Scaffold

As was mentioned above, for Scaffold versions 3.2.0 and higher, the installation packages will contain X! Tandem version 2010.12.1.1. Information about this version is available from The GPM at:

<http://thegpm.org/TANDEM/index.html>

Please note that this version of X! Tandem may give different results. Users who need to reproduce results seen in prior versions of Scaffold may wish to reinstall the old version of X! Tandem. To do so, please rename the X! Tandem executable file found in the programs folder under the Scaffold installation directory so that the new version can be restored later. For example, on a Windows system, the file is called **tandem_win.exe**, which could be changed to **tandem_win_new.exe**. The old version can be downloaded from one of the following links, depending on your operating system:

[tandem_win.exe](#)

[tandem_linux.exe](#)

[tandem_intel_mac.exe](#)

[tandem_mac.exe](#)

Place the file into the programs folder under the directory in which Scaffold is installed.

If you have any questions, please contact:

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