Release Notes for FELIX Desktop 2002

Introduction

This document contains important information for users of FELIX Desktop 2002. Please see *Contents* on page 2.

What's New in FELIX Desktop 2002

♦ Compared to FELIX 2001, we've ported and improved the Assign and Autoscreen modules from Felix 2000 to Felix 2002.

♦ Compared to FELIX 2000, we've added functionalities for processing and analysis of 1D spectra to the Autoscreen module.

♦ Compared to FELIX 2000, we've added a new feature to Autoscreen that takes advantage of a series of 2D titration spectra and provides more reliable peak tracing and measurement of chemical shift changes.

♦ The original separate DOS command window of FELIX has been replaced by a docking graphic output window integrated in the main window.

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General

FELIX Desktop 2002 release inherits most of the functionalities from FELIX 2000 for the UNIX operating system, including the following modules:

♦ 1D, 2D and ND processing

♦ Assign

♦ Autoscreen

The following special-purposed modules (and several commands that were specifically designed for these modules) are not available in this release:

♦ Model

♦ Analytical

New functionalities and improvements have been introduced to FELIX Desktop 2002. They are detailed in *"Major Changes to FELIX*

System Requirements

OS: Window 98 (Second Edition), Windows NT (Service Pack 6), Windows 2000 (Service Pack 2), Windows XP

CPU: 300 MHz and up

Disk space: Minimum required, 200 M Bytes

Memory: 128 M Bytes and up (256 M Bytes preferred)

> **Note:** FELIX spreadsheets need a lot of memory. Displaying long tables; e.g., peak tables containing tens of thousands of peaks), requires at least 256 MB of memory (RAM).

Installation Instructions

New FELIX 2002 Users

1. Insert the FELIX installation CD into your CD drive. From Window Explorer, double-click the *setup.exe* file on the CD.

2. Follow the installation wizard to install FELIX 2002 and the License Pack step by step. At the last step, deselect **Launch License Installer.** Click **Finish**. If you are installing FELIX on a machine running Windows 98 you'll need to reboot the computer. Please see *All users* on page 4.

3. To install a demo license, select **Start** (at low-left corner of the screen) > **Programs** > **Accelrys Felix 2002** > **Demo License Installer**.

FELIX 2002 Beta Users

Before installing the FELIX 2002 commercial release, uninstall the Accelrys License Pack and FELIX 2002 Beta.

1. From the Windows taskbar, select **Start** > **Control Panel** > **Settings** >**Add/Remove Programs**. Select **Accelrys License Pack** from the list and click **Add/Remove**. Follow the screen prompts to remove the program.

2. Repeat the process to uninstall FELIX 2002 Beta. When you are finished, you may install the FELIX 2002 commercial release.

> **Note:** If you fail to uninstall the existing Accelrys License Pack before installing the FELIX 2002 commercial release, you may encounter a problem launching the FELIX 2002 executable. This is caused by a licensing problem.
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> To work around this problem, uninstall the existing Accelrys License Pack as described above. Then install the new version of the Accelrys License Pack from the **support** directory of the FELIX 2002 Commercial Release CD.

All users

PCs running Windows 98 cannot be configured as license servers. The License Pack can only be configured as a client on Win98. Accelrys supports running the license server on Irix, Sun, IBM, Linux, WinNT, Win2000 and WinXP only.

Starting FELIX 2002

Do one of the following:

♦ Double-click the **Felix** icon on the desktop.

♦ Select **Start** > **Programs** > **Accelrys Felix 2002** > **Felix 2002** from the Windows taskbar at the bottom-left of the screen.

Major Changes to FELIX 2002 Compared to FELIX 2001 Desktop Release

♦ Added an option to the **File/Close** command that closes the spectral window.

♦ Added new commands, **View/Output** and **View/Command Input**, to reopen the output and command windows when they are closed.

♦ Added an option to automatically arrange the spectral and table windows. This option can be turned on or off by selecting the **Preference/Frame Layout** command. When turned on (the default setting), the spectral and table windows are automatically tiled, cascaded, or arranged whenever a new window is opened.

♦ The initialization macro *init.mac* (located in %ACCELRYS_ FELIX2002%\macros\mac\, where ACCELRYS_FELIX2002 is your installation folder) has been split into two macro files. The first one, *init.mac*, is executed by FELIX before launching the graphical window; the other, *init_win.mac*, is executed by FELIX after launching the graphical window.

♦ For the table frames (windows containing a spreadsheet), some new commands are added to take better control of their appearances:

tbl zero
closes all table frames

tbl resize tblname x0 y0 xsize ysize
resizes the table frame

tbl move tblname x0 y0
moves the table frame's origin to x0 and y0.

tbl front tblname
activates the table frame as the current window

tbl exist tblname symbol
Checks if a table frame exists or not

♦ The size of the main window is registered and persistent across sessions.

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♦ The command **`fra who`** has been extended to the followwling syntax:

```
> fra who ID_of_active_frame [count_of_frames max_ID_of_frames]
```

where the optional symbols **`count_of_frames`** and **`max_ID_of_ frame`** return the count of spectral frames and the maximum ID number of the frames.

♦ The syntax to specify a toolbar icon has been extended to allow user to specify callback control, specify the command description on the status bar, and to add licensing control, similar to the syntax that specifies a menu item. The new syntax is exemplified in the following:

```
> icon draw.icon "ex experselect 2" "Draw" NULL "Plot the highlighted experiment." 1 NULL optnd
```

♦ Improved the **`tbl dbc`** command so that you can specify callback control similar to menu or tool icon commands:

```
tbl dbc <table_name> <command> [<callback_control>]
```

If default or **`callback_control`** = **0**, the <**`command`**> is called only once with the proper parameters (**`item_num`**, **`row_num`**, **`col_ num=0`**). If <**`callback_control`**> **!=0**, the <**`command`**> is called twice; the last time with (-**1**, -**1, 0**) as parameters.

♦ Added an option to the command **`xyp fit`** so that **`xyp fit 8`** fits the xy pairs to a rectangular hyperbolic function

$$f(x) = A0*(x/(x+A1)).$$

This function is useful for calculations such as the dissociation constant (Kd) of protein/ligand binding.

♦ For all the ND processing commands (Process/2D Processing, etc.), a new button is provided in the EZ nD DATA PROCESSING dialog box next to **Output Matrix Filename**. It allows you to navigate to a certain folder and then provide a matrix filename.

♦ Improved the **option** (combo) box syntax so that the options can be specified in a text file, similar to the list box. In a menu (*.mnu*) file, you can specify a combo box in the following syntax:

```
> *pf cx cy cwidth num_ops file_name #_select_line select_line [num_ops_to_use] [(depend)]
```

where **`cx,cy`** are the starting points of the combo box, **`cwidth`** is the width, **`num_ops`** is the number of options expected, **`file_ name`** is the filename of the text file where the options are listed,

`#_select_line` is the symbol to accept the number of the option you select, and `select_line` is the symbol to receive the contents of the option you select. Optionally you can specify `num_ops`_to_ use as the number of options to display from the file (which maybe equal or smaller than `num_ops`), and the dependency of the combo box.

Most of the length list boxes in the dialog boxes relevant to the Assign module have been replaced by combo boxes specified in this new syntax.

Major Changes to FELIX Desktop 2002 Compared to FELIX 2000 for UNIX

♦ The maximum number of loops and nests of loops in macros have been doubled to 128 and 16 respectively. The maximum number of (if-then) conditions has been doubled to 256.

♦ In FELIX 2002, you can manipulate a spreadsheet as you would treat a spectral frame. Hence you can use the command '`mnu p <mnu_file>`' to display a dialog for the spreadsheet. The old command '`mnu s <table_name> <mnu_file> <x> <y>`' can still be used and FELIX simply ignores the `<table_name>`.

♦ Real-time phasing is changed to be macro-based. The following new command is added:

piv <flag>

to turn on/off the display of the pivot (default or 1 = **on**. 0 = **off**). A new reserved symbol '`pivot`' is used to remember the current pivot point as data point number.

♦ 2D display projections can show levels and zero lines similar to the 1D display. If using the workspace buffer for projection, complex data is okay and can display the imaginary part.

♦ The toggles in the FELIX 2002 menus and the combo box in the tool bar are automatically updated based on the values of their dependent symbols. In previous versions of FELIX a command '`cmd <symbol> <value>`' is used to explicitly update the display of the toggle or combo box.

- ♦ The leading spaces before a command issued from the command bar are automatically ignored. If an empty command is typed, the text port shows a blank line. Use the **Up** and **Down** arrow keys to browse the past issued commands. Up to 10 commands are saved from the command bar.

- ♦ FELIX 2002 provides real WYSIWYG printing facilities, including the following subcommands:

  `hcp setup` for *printer page setup*

  `hcp preview` for *print preview*

  `hcp` for *printing*

- ♦ The parameters used for controlling the spectral display are used for printing as well. The separate set of parameters, specifically relating to the `hardcopy copy` command in previous versions, is obsolete.

- ♦ In FELIX 2002, user symbol `'pltusr'` is used to toggle between '**page**-**filling**' mode and the '**user**-**defined size**' mode for both display and hardcopy. If `pltusr=1`, `xzero`, `yzero`, `xsize`, `ysize` controls the size of the spectrum box in inches.

- ♦ For 2D plots, the width of the projection part does not shift the box location. In addition, if the screen frame is smaller than user defined size, then only part of the spectrum will be seen. In previous versions, FELIX tried to shrink the size, which seems to be less logical.

- ♦ The same hardcopy commands also work for a spreadsheet view. The item numbers and column titles are printed together with the data.

- ♦ `tym` writes *only* to the status bar instead of to both the text port and the motif text port as in previous versions. This prevents outputting too much information to the text-port in cases like `'Cursor Value'`.

- ♦ The '**Auto Scale**' icon is changed to a toggle that switches between the fill-in mode and in-scale mode for 2D and ND spectral display.

- ♦ In the **File/New** command an option was added to choose to open a new, empty window, in addition to the previous choices to build a new matrix or *.dba* file.

- ♦ If an annotation file is already defined users have three options: to use it, not use it, or to open another file when using the **Edit/ Annotation** command.

- ♦ Windows allows for spaces in a file or folder name. To avoid potential problems in FELIX macros:

  All symbols that hold pathnames or file names are single quoted.

  The filenames passed to the **'sys'** command are double quoted, for example:

```
sys 'copy "&xxpath&xxname" "&xxpath&yyname"'sys 'del/f/q "&xxpath&xxname"'
```

- ♦ Some new subcommands are added to achieve the common file manipulations:

```
sys del '<filename>'
sys copy '<from_file>' '<to_file>'
sys rename
'<from_file>' '<to_file>'
                              etc.
```

Note: Although entering spaces in the path or filename is generally okay for FELIX 2002, be cautious with it since the FELIX database does not normally allow for spaces in an element.

- ♦ When launched, FELIX 2002 reads the file '*felixrc.ini*' to obtain the pathnames for macros, menu file, database schema etc. This file is located in the folder where FELIX is installed. The folder name is registered in a system environment variable called 'ACCELRYS_FELIX'). Note that '*felixrc.ini*' replaces the .*felixrc99* file used in previous versions.

- ♦ By default, the current working folder of FELIX 2002 is where FELIX is installed. To change it to another folder, change the properties of the shortcut (the **Felix** icon) on the desktop.

- ♦ After FELIX is started, every time a database file (.*dba* file) is opened, the current working directory is set to that folder. If other paths are relative ones, they are also changed. If they are absolute ones, they remain unchanged. To change the current working directory select **Preference/Directories** from the FELIX 2002 toolbar.

- ♦ The *.icon* files used to define the toolbar icons are 16x15 16-color bitmap files. Such files can be generated with programs such as Microsoft Paint or Microsoft Visual Studio.

- ♦ All dialog box components can have dependency, exit status, and associated commands, except for the **File/Open** command.

- ♦ While a user-defined button can have any exit value, the following exit values have been reserved for the following buttons (although the title can always be changed by you):

  Cancel (exit value = 0) restores all relevant symbols to their initial values. Clicking the [**X**] closes the dialog just like **Cancel**, but there is no associated command.

  Reset (exit value = -1) restores all relevant symbols to initial value, but does not close the window.

  Apply (exit value = -2) saves the values for all relevant symbols and does not close the window.

  Any button with exit value = -9 does not close the window.

  With this flexibility, some original '**Reset**' buttons executed by macro commands can now be controlled by the dialog box itself. **Reset** and **Apply** buttons also can have associated commands.

- ♦ In contrast to a modal dialog box, which locks the main window until it is closed, a modeless dialog box does not prevent users from accessing the main window menus and items.

- ♦ For a modeless dialog, none of the buttons will close the dialog box. A command `'mnu r <name>'` is expected to explicitly close the dialog box (`<name>` is the mnu file name without the suffix `'.mnu'`).

- ♦ Clicking the [**X**] button on the dialog box closes it in the same way that clicking **Cancel** closes a modal dialog box. In all other ways, a modeless dialog box works the same way as a modal one.

- ♦ Modeless dialog boxes are no longer associated with a specific frame; rather, they are shared by all frames.

- ♦ The first time a dialog box is displayed, it is located near the center of the main window. The next dialog box is always displayed in such a way that its upper-left corner is at the same location of the previous dialog before it was closed.

♦ Some changes to the syntax of the dialog box definition (*.mnu*) files:

Label:

```
*c cx cy clength 'Label'
```

The `clength`, number of characters in Label, is ignored and width is automatically determined.

Button:

```
*b[t] cx cy cwith 'Label' index [(depend)
```

If the optional `'t'` is not specified, the button is drawn with normal height (extending by 1/3 character height in up and down directions). If `'t'` is specified (`'*bt'`), the button is drawn thinner so that it fits line by line display.

Option/Combo box:

```
*p cx cy cwidth num_ops  'opt1' 'opt2' ... symbol [num_ops_to_use] [(depend)]
```

The width of the combo box, `cwidth`, is more strictly enforced than in previous versions of FELIX.

Also, a new feature is added so that you can specify the actual number (`num_ops_to_use`) of options to display. This is useful when the maximum number of options is fixed but the actual number of options to display is determined at run-time.

File Open/Save:

```
*o cx cy cwidth cheight <# lines> <extension> <dir> <filename>
```

♦ In previous versions of FELIX, the layout is controlled by `<#lines>` and `<cheight>`. In FELIX 2002 the `<#lines>` is ignored, but the `<cheight>` is used to control the total height of the combo. The actual height of the file list is about `<cheight>` - 5 lines (but is not equal to the displayed lines). If less than 8 lines, the `<cheight>` is set to 8.

♦ In previous versions of FELIX, the **OK**, **Filter**, and **Cancel** buttons are automatically drawn and the user cannot control them. In FELIX 2002, you can specify the buttons explicitly, otherwise the **OK** and **Cancel** buttons are automatically added.

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♦ In FELIX 2002, symbols (not symbol values as in previous versions) must be used for `<extension>` and `<dir>` if those symbols are to retain the changed values (i.e., new extension and new path selected by the user). If values are used for <extension> and `<dir>` new values entered will not be retained.

Slider:

```
*a cx cy cwidth minsym maxsym decimal orient dragCB symbol 'label' [edit_width] ["command"]
```

♦ You can use `<edit_width>` to specify the width of all the edits. The default width is 6 characters.

♦ A new command to shift dialog components vertically is:

`*d cy`

It moves all the dialog components below this line by `cy` lines down (if `cy` is positive) or up (if `cy` is negative). Note the number of lines to move accumulates in the same *.mnu* file if multiple `*d` lines are specified. A line of "`*d 0`" terminates the shifting.

♦ A new menu item is added to the **Preference/Export/Reference** command. This item allows you to export the references from one frame to another.

♦ The **Preference/Macro Debug** menu item was added, allowing users to set the debugging options for macros.

Task List When Migrating Macros from FELIX 2000 for UNIX

Note: You do not need to change a macro for FELIX 2001 Desktop Release when migrating to FELIX 2002.

When migrating macros and .mnu files for FELIX 2000 for UNIX, in addition to observing the changes to FELIX 2002 as described above, you may need to make the following changes:

♦ In the path names, characters '/' must be changed to '\'. If a symbol is to represent a path or filename, add quotation marks around it to preserve possible spaces in the path or filename. Although spaces in path or filename is generally okay for FELIX

2002, be cautious in using spaces in the file path or filename, since the FELIX database does not allow spaces in an element.

♦ The UNIX commands used in the FELIX `'sys'` commands (e.g., `"sys '/bin/cp &file1 &file2'"`) must be replaced by the similar DOS commands.

♦ Real-time phasing is changed to be macro-based. So, replace `'rph'` with the corresponding macros (e.g., *rtphase.mac*)

♦ Real-time polynomial definition is now macro-based. Replace `rpl` with the corresponding macros (e.g., *rtbasepoly.mac*)

♦ Behaviors of modeless dialogs have small changes so macros using them may need to be revised. At least, the command `'mnu r xxx'` must be explicitly used to remove the dialog. Clicking buttons won't automatically close the dialog as in previous versions of FELIX.

♦ The *.icon* files used to define the tool bar icons are 16x15 16-color bitmap files. The *.icon* files from a previous FELIX version may not be reused. You can redesign your own icon files using programs such as Microsoft Paint or Microsoft Visual Studio.

♦ Macros that use DOS commands to display file contents must be changed, because the DOS command messages are no longer visible. You can use FELIX commands to open the file (`opn`), read (`rea`) and then display (`ty`) each line therein.

Problem starting FELIX 2002 with Accelrys License Pack 5.0 and Accelrys Materials Studio installed on a PC

Problem:

On a PC running Windows NT or higher meeting all four of the criteria below:

1. Installed FELIX 2002

2. A copy of License Pack 5.0 (due to an installation of Accelrys Materials Studio on the same PC)

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3. License Pack 5.0 is set up as a license server via the **Start > Programs-Accelrys License Pack 5.0 > Configure Licensing** option

4. Attempt to register and start the license service

When trying to start FELIX 2002, an error dialog appears that starts with the text:

```
Cannot connect to license server
The server (lmgrd) has not been started yet, ...
```

Cause:

For some installations that meet the above criteria, the "Configure Licensing" program will successfully register, but not start the license server service.

Solution:

Using the Services control panel (found under "Administrative Tools" in the control panel on Windows 2000 and XP):

1. Find the license service entry that you defined (default value is "Accelrys License Server").

2. Select the entry so that it is highlighted.

3. Using the "Action" menu or the right mouse button, select **Start** to start the service.

Contacting Accelrys

Bugs and comment should be reported directly back to Accelrys by email to Steve Unger at swu@accelrys.com.