FELIX 2002

Getting Started

MARCH 2002

*All updated documentation (**User Guide**, **Tutorials**, and FELIX **Command Language Reference**) for the latest release of FELIX is available at the Accelrys website documentation library:*

http://www.accelrys.com/doc/life/index.html

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Contents

1. Welcome to FELIX 2002

What does FELIX do?

FELIX 2002 is an interactive program for processing, displaying, and analyzing data acquired on nuclear magnetic resonance spectrometers (NMR).

A complete NMR data processing and analysis program, FELIX provides you with tools for efficiently transforming NMR data of almost any dimensionality and for processing, displaying, storing, and retrieving the resulting spectral information.

FELIX is flexible and efficient. It can run either as a menu-driven graphical interface or as a concise and powerful command-driven program (via the FELIX Command Language: FCL). In addition, the FELIX macro processor enables you to automate lengthy and complex processing procedures (for example, routine or ND data processing). FCL is powerful enough to permit you to create your own menus and user interface or to customize the existing menus.

The quantity and variety of data that FELIX handles, ranging from peak integrals to assignment names of ND peaks, demands powerful data storage and management features, which are provided by the FELIX database. The database is accessible from many FELIX functions (e.g., the peak picking and assign interface), from the command line, or from within macros. The tools provided by the database allow you to quickly store data temporarily or permanently in files, to display the data as lists, and to edit the spectral information using a table interface. The database also sorts data into lists according to user-defined criteria and can compare lists for similarities or differences.

Features of FELIX 2002

FELIX's major functions include general features for NMR spectral processing and basic analysis, and specialized module features for biomacromolecular resonance assignment and receptor-ligand binding analysis. You may need to obtain ND, Assign, or Auto-screen license privileges to access the special features of FELIX.

General features

- Platform-independent data file transfer between machines without file conversion.
- Direct reading of native spectrometer FID files from different vendors (Bruker, Varian, JEOL).
- Zero-filling of data sets.
- Linear prediction of the first and last points of an FID, with or without root reflection.
- Linear prediction of last points using mirror image methodology.
- DC offset correction.
- Window functions: exponential, sinebell, sinebell squared, skewed sinebell, skewed sinebell squared, Gaussian, trapezoidal, Kaiser, and convolution difference.
- Fourier transforms: complex fast Fourier transform (FFT), Bruker FFT, inverse FFT, real FFT and digitally oversampled FFT for Bruker data.
- Generation of complex data from real data for phasing using Hilbert transform.
- Baseline correction with automatic and manual baseline point selection; also cubic spline and polynomial baseline correction.
- Solvent suppression using time domain convolution, LP-SVD, and polynomial fitting.
- Spectrum phasing: automatic, real-time, and manual.

- Data buffer stack for easy storage and retrieval of free induction decays (FID's), spectra, and other plots, allowing comparison and point-by-point arithmetic operations between pairs of data buffers.
- Integration of the full spectrum of segments and integral values displayed on plot (and stored in database).
- Automated 1D line fitting for obtaining accurate integrals of noisy or poorly resolved data.
- Automatic or manual peak picking of 1D and 2D data; labeling of picked peaks with axis units.
- Enhanced peak picking using example peaks.
- 2D peak fitting and peak modeling.
- J-coupling extraction for 2D DQF and E-COSY spectra.
- J-coupling extraction based on heteronuclear E-COSY, FIDS, FIDS-E-COSY, and DQ-ZQ methods.
- Easy page setup, print preview and printing.
- Display features that include spectrum expansion, real plots, imaginary plots, and real/imaginary plots for 1D data or 1D slices of 2D data.
- Menu access for rapid, customized 1-D processing.
- Matrix storage of two-dimensional (2D) data for easy access to t_1 and t_2 data vectors.
- Supplied macros for simplified processing of states, TPPI, states-TPPI, and N/P 2D data.
- Enhanced contour plot for accurate and fast representation of peak intensity in two dimensions.
- Intensity plot for fast 2D data display of positive and negative peaks.
- Volume integration in two dimensions.
- Database tools for storing and correlating peak assignments.
- Tile plot to display isolated sets of overlapping peaks, simplifying identification of related peaks.

- Correlated cursors to permit accurate comparison of peak positions in several graphics frames at one time.
- Flexible frame connection to analyze multiple *n*D spectra concurrently.
- Keypad navigation within plots.
- Lists that allow you to sort and compare information (e.g., cross peak data from the database).
- Matrix compression to reduce 2D data set storage requirements, with minimal loss of spectral information.
- Importing processed data from other processing / analysis software: NMRCompass, NMRPipe, Bruker, and Varian.
- Flexible restraint generation tools for NOE-distance, NOE-volumes, ^{3}J-dihedral, and ambiguous NOE-distance and NOE-volume categories—either in Discover / DG-II or X-PLOR format.
- Relaxation-time analysis for 2D heteronuclear data.
- Table interface to the database.

Special features for ND processing

The ND license allows you to access the following capabilities in addition to the general features in FELIX 2002.

- 3D transformation macros for states, TPPI, states-TPPI and N / P data.
- Plane transformation for 3D states, TPPI, states-TPPI and N / P data.
- 4D transformation macros for states, TPPI, states-TPPI and N / P data.
- Distributed processing for 3D and 4D transformation.
- Rapid “bundle mode” access to matrix vectors.
- Convenient display and analysis of 2D planes in 3D and 4D matrices from any direction.
- Keypad navigation between planes.

- Slider control for plane selection.
- Convenient access to 1D vectors from 3D and 4D matrices.
- 3D / 4D peak picking and volume integration.
- Enhanced peak picking using example peaks.
- 3D / 4D cross peak filtering.
- 3D / 4D cross peak modeling.
- Matrix compression to reduce 3D / 4D data set storage requirements, with minimal loss of spectral information.

Assign module features

- Comprehensive features to organize the assignment project in a database.
- Define up to 12 spectra in one experiment.
- Overlay multiple contour plots in real time.
- Overlay multiple peak entries on contour plots.
- Tile and strip plots from frequency clipboard, spin systems (patterns), or prototype patterns.
- Display frequency clipboard or frequencies of spin systems (patterns) or prototype patterns on plots.
- Automated routines for detecting spin systems via systematic search in:
- 2D TOCSY, COSY, and / or NOESY spectra
- 3D homonuclear spectrum (e.g., 3D TOCSY-NOESY)
- 3D ^{15}N HSQC (or HMQC)-TOCSY spectrum
- 2D ^{15}N-^{1}H HSQC and 3D ^{15}N HSQC-TOCSY spectra
- 3D HNCO, HNCA, and HN(CO)CA spectra
- 3D CBCANH and CBCA(CO)NH spectra
- 2D ^{15}N-^{1}H HSQC and 3D CBCANH and CBCA(CO)NH spectra
- 3D HNCO, CBCANH, and CBCACO(N)H spectra
- 3D HNHA, CBCANH, and CBCA(CO)NH spectra

- 4D HNCAHA and HACA(CO)NH spectra
- 3D HCCH-TOCSY spectrum
- 3D H(CC-TOCSY)(CO)NH spectrum
- Automated routine for detecting spin systems via simulated annealing in 2D TOCSY, and 2D COSY and / or 2D ^{13}C-^{1}H HSQC spectra.
- User-tailorable semi-automated routine to exploit virtually any combination of heteronuclear double and triple resonance experiment to detect spin systems.
- Fuzzy algebra-based procedures for verifying new patterns.
- Library-based identification of patterns and frequencies using all-atom matching or the C-C combined chemical shift expectation value method.
- Sequential connectivity detection routine based on:
- 2D NOESY spectrum
- 3D homonuclear NOESY spectrum (e.g., 3D NOE-NOE)
- 3D ^{15}N HSQC (or HMQC)-NOESY spectrum.
- Triple resonance spin systems.
- Rule-based approach to make sequence-specific assignments.
- Simulated annealing-based approach to make sequence-specific assignments.
- Tools to visually inspect and manually override the results of automated methods in all stages of the assignment procedure.
- Point-and-click manual assignment of frequencies or peaks.
- Automated peak assignment of up to 4D spectra based on assigned patterns for NOE and / or COSY type spectra; generating and storing ambiguous (multiple possible) assignments.
- Chemical shift index calculation based on H, C, and C chemical shift libraries.
- Tool for generating reports about the assignment of patterns.

Autoscreen module features

- Comprehensive features to organize a 1D or 2D SAR by NMR-like project in a database.
- Unlimited number of 2D ^{15}N-HSQC spectra can be processed, plotted, and reviewed.
- Unlimited number of 1D spectra can be processed, plotted, and reviewed.
- Automated processing of spectra based on parameters from a control spectrum.
- Novel algorithm for automated phasing of *N*D spectra.
- New algorithm for automated baseline correction.
- Innovative scoring algorithms that provide reliable peak-matching and -identification in situations where peaks in a reference spectrum disappear or additional peaks appear in spectra of protein-ligand complexes.
- Use of peak shape, including both peak widths and heights, for reliable peak matching and scoring.
- New progressive peak tracing (PROPET) algorithm that provides more reliable peak matching by taking advantage of titration spectra.
- Automated peak matching and scoring of an unlimited number of test spectra.
- Tools for overlaying multiple contour plots in real time and displaying peak displacements.
- Tools for defining and using a selected subset of peaks (region of interest) for scoring.
- Tools for generating reports about interesting spectra (high-affinity ligands) and interesting peaks (binding subsites) and for K_d fitting.
- Connection to Insight II to display molecular structure of ligand and protein.
- Automated coloring of peak displacements on protein surface displayed in Insight II.

- Exporting scores to Cerius^2 study tables for further analysis using QSAR tools.
- Clustering experiments and peaks for identifying individual binding subsites in a protein.

2. System Requirements and Licensing Options

System requirements and recommendations

Minimum system requirements for FELIX 2002are:

- Windows 98, NT, 2000 or XP
- 300 MHz CPU speed
- 200 MB hard disk space
- 128 M Bytes (256 M Bytes or more recommended)
- Standard 2-button mouse

Attention to the following areas will improve performance:

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).

CPU Speed
The faster the floating point performance the better.

Display Resolution
The higher the resolution, the better. A resolution in the range of 1280 x 1024 is optimal but is not required.

The software license

This software release is distributed with FLEXlm license management software. FELIX 2002 must be licensed to run properly.

Accelrys offers two types of licenses:

A demo license
If you received a demo password with your FELIX 2002 ship-

ment, the demo license lets you use the software until you can install the normal license. A demo license allows access to FELIX 2002 for a limited time only.

A license file for use with a license server
The license server may be the local machine where you have FELIX installed or a remote machine where a license file is already installed.

The following information is meant to provide a brief overview of the various licensing options. For more detailed information, please see the *Accelrys License Pack (Version 3.7/3.8/3.9)* included in the FELIX 2002 package.

The program modules

Accelrys offers four licensing options for FELIX 2002:

FELIX 2D
This includes all of the basic FELIX processing and analysis functionality for both 1D and 2D data.

FELIX ND
This option adds the capability to process and analyze higher dimensional data such as 3D and 4D.

FELIX Assign
This option allows you to run the Assign module, a unique package for computer-assisted assignment of 2D, 3D, and 4D NMR spectra of proteins and nucleic acids

FELIX Autoscreen
This option allows you to run the Autoscreen module, a specialized package for automated processing and analysis of receptor/ligand binding 1D or 2D NMR data.

Once you have installed **FELIX** you can determine which version you have licensed. To do so, run FELIX 2002. In the main window, click the **File/Licenses** command. FELIX displays a dialog box describing the license. For example, if the **ND Mode** item is checked, you have the FELIX ND license feature, with the 3D/4D capabilities enabled. Otherwise, the ND featuers are not available to you.

3. Installing the FELIX 2002 Software and License

This chapter gives step-by-step instructions on how to install the FELIX software as well as how to install and configure the licensing software.

Note

If you have a pre-release (beta) version of FELIX 2002 on your PC you should uninstall both the Accelrys License Pack and the FELIX software before continuing. See "Uninstalling the License Pack software and FELIX" on page 15 to learn how to remove the previous installation.

If you have FELIX 2001 installed on your PC, you do not have to uninstall it if you would like to keep it on your machine.

Installation instructions

Accessing the FELIX 2002 installation utility on the CD-ROM

1. Exit all Windows programs to avoid conflicts.
2. Insert the FELIX 2002 installation CD into your computer's CD drive.
3. Double-click the **My Computer** icon on the desktop.
4. Double-click the icon for your CD drive.
5. Double-click the *setup.exe* file on the CD drive.
6. Follow the instructions on the screen.
7. When asked if you want to launch the License Pack Utility follow the instructions below depending on which type of license you want to install.

The installation of the license will vary depending on the type of license file you are using. If you have received a demo license then you may choose to install that initially in order to start using FELIX 2002 right away. You may also choose to install the full license using either a regular license file on you local PC or by using a remote license server.

A. Install a demo license using a demo password

Use this option if you have a demo password and do not want to install the full license at this time. This option allows FELIX to operate for a limited time only.

1. During installation FELIX gives you the option to launch the License Pack Utility. Leave the box marked **Launch License Pack Utility** checked. When the license installer presents two different options to license the software, select the **demo password** option.
2. Enter the demo password in the space provided. Note that it is case sensitive, and must be entered exactly as provided to you.
3. Click **Next** to install the license and finish the installation.

B. Using a remote license server

Use this option if you have a license server already set up on a remote machine and you want to use the license on the remote machine.

1. During installation FELIX gives you the option to launch the License Pack Utility. Leave the box marked **Launch License Pack Utility** checked.
2. When the license installer presents two different options to license the software, select **Configure connection to remote license server**.
3. Enter the license server to use in the format "`port@host`". The default port used by Accelrys is 1715.

   For example, if the server name is "`myserver`" enter the License Server information as `1715@myserver`.
4. Click **Next** to configure the license and finish the installation.

C. Install a regular license file.

If you have already received your license file and you do not have an existing license server, you can use the License Pack Utility to set up this machine as the license server.

1. During installation FELIX gives you the option to launch the License Pack Utility. Leave the box marked **Launch License Pack** unchecked and click **Next**. (If you previously checked it, click **Cancel** now.
2. Click the Windows **Start** button.
3. Select **Programs/Accelrys License Pack/Configure Licensing**.
4. Select **Configure Licensing on this machine**.
5. Browse to your license file and select it.
6. Click **Next**. The next screen shows the results of the license installation.
7. Click **Next** again. The options for registering and starting a license server are displayed.
8. In most cases you can select the first option to start the license server at the end of the installation and click **Next**.
9. Click **Finish** to exit the License Pack Installer.

For more detailed information, please see Chapter 3, “License Pack for Windows systems” in *Accelrys License Pack (Version 3.7/3.8/3.9), included in the FELIX 2002 package.*

Installing/updating the license file

In most cases the license will have been installed as part of the FELIX installation procedure described above. However, if FELIX fails to start up properly and you suspect a license problem, you can use the following procedures to update the license file.

Follow the steps below to install the type of license you need.

A. Installing a demo license

If you received a demo password you can use it to install a demo license and enable the program operation for a limited time.

1. Click the **Start** button
2. Select **Programs/Accelrys Felix 2002/Demo License Installer**. The installer will prompt you to enter the demo password you received.

Caution

The password is case sensitive. Make sure to enter it carefully.

B. Using a remote license server

If you have a license server already set up on a remote machine you may choose to connect to that machine to install the license.

1. Click the **Start** button.
2. Select **Programs/Accelrys License Pack/Configure Licensing**.
3. Since you want to set up this machine as a client to a remote server, select **Configure connection to remote license server**.
4. Click **Next**.
5. Enter the license server to use in the format "`port@host`". The default port used by Accelrys is 1715.

   For example, if the server name is "myserver" enter the License Server information as `1715@myserver`.
6. Click **Finish** to exit the License Pack Installer.

C. Using this machine as the license server

If you have already received your license file and you do not have an existing license server on a remote machine, you can use the License Pack Utility to set up this machine as the license server. If you receive a new license file you can use this procedure to install the new license file on this machine.

1. Click the **Start** button.

2. Select **Programs/Accelrys License Pack/Configure Licensing**.
3. Select **Configure licensing on this machine**.
4. Browse to your license file and select it.
5. Click **Next**. The next screen shows the results of the license installation.
6. Click **Next** again. The next screen shows the options for registering and starting the license server.
7. In most cases you can select the first option to start the license server at the end of the installation and click **Next**.
8. Click **Finish** to exit the License Pack Installer

Uninstalling the License Pack software and FELIX

If you have a pre-release (beta) version of FELIX installed on your PC, you should remove the Accelrys License Pack and then remove FELIX before installing FELIX 2002.

Removing the License Pack utility and FELIX

1. Click the **Start** button.
2. Select **Settings/Control Panel**.
3. Double-click the **Add/Remove Programs** icon.
4. Select the Accelrys License Pack item in the list and click **Add/Remove**.
5. When prompted to remove the program, click **Remove**.
6. The **Add/Remove Programs Properties** menu should still be displayed. If not, redisplay it using steps 1-3.
7. Select the FELIX item in the list and click **Add/Remove**.
8. Select the option to **Remove FELIX**.
9. When prompted, click **Remove** to uninstall the FELIX program.

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4. The FELIX 2002 Interface

To enhance the program's utility without compromising its flexibility, FELIX starts up with an interactive menu-driven interface plus a command enter window. The menu interface reduces the need to memorize a large list of FELIX commands and provides access to the data-processing and analysis utilities using intuitive descriptions and a mouse-driven cursor. The capability to enter commands (Felix Command Language, or FCL) interactivly provides experienced users with direct access to the FELIX command statements.

This chapter focuses on the interactive menu-driven interface.

Note

Advanced users should consult the *FELIX Command Language Reference Guide* for more in-depth information about FELIX capabilities.

You can view and print the online Command Language Reference Guide at this address:

http://www.accelrys.com/doc/life/index.html

Click the **Felix** link and navigate to the document.

If you are prompted for a username and password, use the following:

Username: **science**

Password: **faster**

Introduction to the menu interface

FELIX contains an interactive menu system for data processing, displays, and spectrum analysis. The menu interface automatically appears when the program starts. The purpose of the menu interface is to simplify NMR data analysis and speed repetitive processing tasks. The menus provided contain most of the functions needed for processing and analyzing 1-, 2-, 3-, and 4- dimensional data.

In this guide we refer to the various menu items as follows:

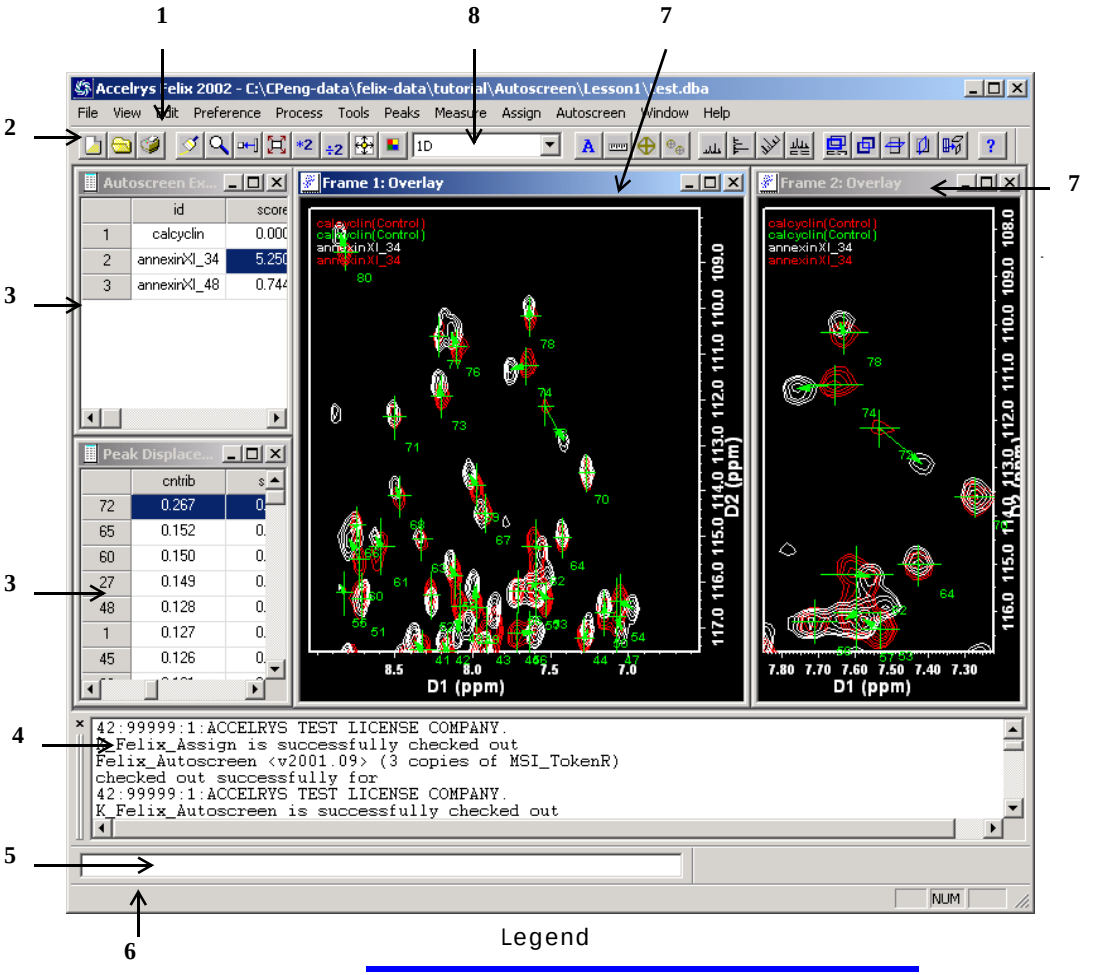
- Horizontal menu: **menu bar**
- Vertical menus: **pulldown** menus
- Vertical lists of menu items appearing when you select an item that ends with an arrow: **pullright** menus

FELIX main window

The FELIX 2002 main window is shown below. It is where you do your work. This window includes these features:

- **Menu bar**
  When you open a vertical menu in FELIX, a pulldown menu displays. Subsidiary (pullright) menus are called from here.
- **Icon bar**
  Activates a function (e.g., print, open file, etc.) when you click on the icon
- **Spectral frames**
  Displays the graphical representation of NMR data
- **Table (spreadsheet) frames**
  View and edit database entries here
- **Output window**
  Results, warning, error messages and other information are displayed here
- **Command window**
  Enter FELIX Command Language (FCL) instructions here
- **Status bar**
  Displays status messages
- **Plot type window**
  Selects the spectrum display type shown in the spectral frame

Figure 1 on page 19 illustrates the main window.



Legend

1	Menu bar
2	Icon bar
3	Table (spreadsheet) frame
4	Output window
5	Command window
6	Status bar
7	Spectral frame
8	Plot type window

Figure 1 FELIX Interface main window

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5. Quick Start

This section introduces some basic features of FELIX 2002. After reading or working through this section, you will be prepared to start working with FELIX.

Quick Start includes five tasks:

For more options on where to learn how to use FELIX, please see Chapter 6, *Getting More Help* on page 53.

Before working with FELIX

Before you begin, be certain that you have:

- Installed a licensed copy of FELIX 2002 on your workstation

  and

- Created a directory on a drive (on your workstation or on a network) in which you have full write permission to create subdirectories and store files.

You should also be familiar with the following:

- The windowing software on your workstation.
- Using the mouse on your workstation.

Typographical conventions

Unless otherwise noted, this guide uses these typographical conventions:

- Names of pulldowns, commands, and other items in the FELIX 2002 interface are presented in **bold** type. For example:

  Select the **File** pulldown.

- Command dialog and file samples are represented in a `typewriter` font. If the dialog is something you must type, it is given in **`bold typewriter`** font. For example:

```
> FELIX -b output scriptfile
```

Starting FELIX 2002

There are two ways to start FELIX.

- Double-click the FELIX 2002 icon on your desktop.
- Click **Start** on the task bar. Then, select **Programs/Accelrys Felix 2002/Felix 2002**.

Note

When you start FELIX, you may have the following two choices depending on if you have run FELIX before and have saved the previous session in an environment file:

- If you've saved the previous session, you are prompted by a **RESTORE LAST SESSION** dialog box. You may select to restore the previous session.
- If you haven't saved a previous session, or if you choose not to restore the previous session, you will define a new .dba file or select an existing .dba file in the next **OPEN DATABASE FILE** dialog box.

Note

FELIX takes its "working directory" from the location of this .dba file. The "working directory" is the default location where FELIX looks for data files, opens matrices, etc.

To change the working directory with FELIX already running, use the **Preference/Directory** command.

You may also set a new default location for the working directory from the Windows Desktop. To do this, click the **Felix** icon using your secondary mouse button (right-click). Select **Properties** from the popup menu. Click the **Shortcut** tab. Then, edit the content in the **Start In:** field to specify the new default working directory.

Processing a 1D spectrum

In this tutorial you will process a 1D NMR data set. Once you are comfortable with the procedures, this task takes approximately ten minutes to complete.

1. Set up for the lesson

Create a folder on your hard drive to store tutorial files. Name the folder **Felix_Practice**. For example:

```
c:\Felix_Practice
```

Caution

Do not put the folder into the same path as the FELIX program files.

Locate the FELIX 2002 directory; it includes the FELIX 2002 executable file, ***felixwin.exe***. If you use the default installation path, the directory is:

C:\Program Files\Accelrys\Felix 2002

If you have trouble locating the installation directory, you can:

Right-click the **Felix** icon on the Windows desktop. Click **Properties**. On the **Shortcut** tab of the popup, note the path listed for the **Target** parameter.

Navigate through the directory structure using the Windows Explorer program. To access Windows Explorer, right-click either the **My Computer** icon or the **Network Neighborhood** icon on your Windows desktop; select the **Explore** option.

Once you have located your installation directory, locate and open the **tutorial** subdirectory (folder). Next, locate the **1D** folder. This folder contains the 1D data used for this lesson. By default, the **1D** folder is located at:
C:\Program Files\Accelrys\Felix 2002\tutorial\1D

Copy the **1D** folder to the **Felix_Practice** directory. (If you have not already created a directory called **Felix_Practice**, please refer to "Set up for the lesson" on page 23.) To copy it quickly, right-click the folder and hold the button down. Next, drag the **1D** folder to the **Felix_Practice** folder and release the mouse button. Select the **Copy Here** option.

2. Start FELIX.

Start FELIX by double clicking the **Felix** icon on your desktop, or by clicking **Start** on the Windows taskbar, then selecting **Programs/Accelrys/Felix 2002/Felix**.

If FELIX prompts you to restore from last session, click **Cancel**.

FELIX displays an **OPEN DATABASE FILE** dialog box. Navigate to your working directory. If you use the default suggestion, this is:**C:\Felix_Practice\1D\Lesson1**.

Enter a new filename (e.g., ***test***) for a new, empty database. When you enter the name of a brand new database file, FELIX creates the file.

By default, where you open the database file becomes the current working folder. To change the working folder select **Preference/Directory**.

Select the **File/Open** command. Set the **File Type** parameter to **Other Data [Bruker, Varian...]**.

Double-click the folder named **1**. This is the experiment directory. From the contents of this folder, select the **fid** file. Click **OK** to confirm the selection. FELIX opens the file in the window.

This loads the data. The graphics frame displays a 32768 point FID, which we can now process.

Routine 1D data processing often consists of removing ***DC offset****, multiplying the FID by an exponential window function, transforming the results into the frequency domain, and phasing the spectrum to obtain pure absorption peaks. Subsequently, baseline roll is removed and the spectrum is integrated. We follow these steps here.*

3. Remove DC offset

Select the **Process/DC Offset** command and choose **Oversample DBC** as **Type**. Click **OK** to perform the DC offset removal.

FELIX calculates a value for the baseline from the last 20% of the data points and subtracts that value from each data point.

4. Apply Window Function

Select the **Process/Window Function** command to obtain a control panel that prompts for a window function. Enter **Exponential** as the Window function and click **OK**.

In the following control panel, enter **0.2** for **Line Broadening** and click **OK** to multiply the data by an exponential window function.

The display is updated to show the results.

5. Fourier-transform the data

Now, transform the data from the time domain to the frequency domain using the oversampled transform (this data was collected as a Bruker oversampled spectrum).

Select the **Process/Transform** command. FELIX determines that the transform type should be **Oversampled FFT**. Click **OK**.

The result is a spectrum in the graphics frame. Notice that the spectrum requires some phase correction. This is most easily applied by first using the phase parameter values from the procs file.

Select the **Process/Phase Correction** command. Set the **Method** to **Parameter** and leave the **Zero** and **First Order** parameters at their current values (136.912 and 14.55447, respectively). Click **OK**.

This should produce an almost perfectly phased spectrum. If you need to adjust the phasing you can use the real-time phase interface.

To activate the real-time phase correction interface, select the **Process/Phase Correction** command and select the **Real-Time** option. Click **OK**.

You can change the pivot point by clicking **Pivot** *and then clicking the desired spectral point. Usually the pivot point is at the lowest end (near the last peak) in the spectrum.*

Use the **REAL TIME PHASING** dialog box to adjust the pivot point, the zero-order phase correction (**Phase0**), and the first-order phase correction (**Phase1**). Change the phase values by sliding either of the sliders left or right. These changes are visible in the display as you make them.

Since this is a modeless dialog, you can still activate the main menu and toolbar icons to adjust the display of the spectrum while the phasing dialog is on.

Repeat this with each correction until you are satisfied with the spectrum, then click **OK** to complete the phase correction.

This removes the real-time phase interface and makes the phased spectrum appear in the graphics frame.

6. Perform the baseline correction

Select the **Process/Baseline Correction** command. Toggle on the **Baseline Point** selection. Leave the parameter at **Auto Pick Points** alone. Click **OK**.

In the next control panel, leave the **Interval** size at 128 and **Maximum Deviation** at 5. Click **OK**.

After FELIX selects the baseline points, it marks their locations with red tick marks at the bottom of the display frame.

In the **BASELINE CORRECTION** dialog, toggle the **Baseline Correction** to **on** and select the **Polynomial** option. Click **OK**.

When the dialog appears that prompts for the **Polynomial** order, keep the default of **5** (fifth-order polynomial). Set the **Interval Width** to **5**. Click **OK**.

FELIX applies the polynomial function to the spectrum.

FELIX re-displays the **BASELINE CORRECTION** dialog. Click **Done** to close it.

7. Integrate and display the data

The last step is to integrate the areas of the peaks and display the integrals as a cumulative sum.

Select the **View/Draw Integrals** command.

*FELIX calculates the integral of all the peaks and displays the integral on the spectrum.If you want to integrate individual peaks, you can use the **Measure/Integral and Volume** command.*

8. Exit FELIX

To exit FELIX, select **File/Exit** to begin the shutdown sequence.

You either leave the **Save Current Session** and **Save Current Database** parameters on, or toggle them to **off**. Then click **OK**.

This shuts down FELIX. If you choose to save the current session and save the current database, FELIX saves the current session and the baseline points or integrals in the database file you selected when the program started.

You should now be familiar with the basic 1D processing features of FELIX and how to navigate through the menu system.

Processing a 2D spectrum

In this lesson you process a 2D matrix, display the spectrum using a variety of standard plotting methods, and assign the cross peaks. You start by processing a 2D matrix using the EZ macros. This lesson takes approximately 60 minutes to complete once you are comfortable with the procedures.

1. Set up for the lesson

*This lesson uses the **2D** tutorial data set. When FELIX processes data it expects to see the data with the same directory structure as existed on the spectrometer. So, in this lesson you will copy a sample 2D dataset to your working directory.*

Once you have located your installation directory, locate and open the **tutorial** subdirectory (folder). Next, locate the **2D** folder. This folder contains the 2D data used for this lesson. By default, the **2D** folder is located at:
C:\Program Files\Accelrys\Felix 2001\tutorial\2D

Copy the **2D** folder to the **Felix_Practice** directory. (If you have not already created a directory called **Felix_Practice**, please refer to “Set up for the lesson” on page 23.) To copy it quickly, right-click the folder and hold the button down. Next, drag the **2D** folder to the **Felix_Practice** folder and release the mouse button. Select the **Copy Here** option.

2. Start FELIX

Start FELIX by double clicking the **Felix** icon on your desktop, or by clicking **Start** on the Windows taskbar, then selecting **Programs/Accelrys/Felix 2002/Felix 2002**.

If FELIX prompts you to restore from last session, click **Cancel**.

FELIX displays an **OPEN DATABASE FILE** dialog box. Type the new filename in the **File name** field to create a new database file.

Where you create or open the .dba file determines your initial working directory.

Navigate to your working directory. If you used the default suggestion, this is:
C:\Felix_Practice\2D\Lesson1.

Type ***file.dba*** in the **File name** field to create a new database file.

Instead of going directly to 2D processing, first we will apply a few 1D processing functions on the first FID in order to get some spectral parameters.

3. Read in the first FID.

Select the **File/Open** menu item. Set the **File Type** parameter to **Other Data (Bruker, Varian...)**. Double click on the **1** folder (the experiment directory) to open it. Locate and click on the ***ser*** file to select it. Click **OK** to open the file.

This file is the first FID of the 2D HSQC spectrum collected on a Bruker spectrometer.

4. Apodize the FID.

Select the **Process/Window Function** menu item. Select **Sinebell^2** as the apodization function.

In the next control panel, leave the default parameters (**512** and **90.0**) and select the **Real-Time** option for **Method**.

*The FID is displayed along with the apodization function in red. You may experiment with different settings of the **wsize** and **wshift** parameters. The effect on the FID is displayed in real time.*

Set the **Window Size** parameter to **512** and the **Phase Shift** parameter to **90**. Then click **Keep**.

The apodized FID is now displayed on the screen.

5. Transform the FID

Select the **Process/Transform** menu item. The default is **Complex FFT**. Click **OK**.

6. Phase-correct the spectrum

Select the **Process/Phase Correction** menu item. In the control panel, select the **Real-Time** option for **Method** and click **OK**.

When the real time phase interface appears, click **Pivot** to select a peak to use for zero-order phasing. Using the mouse, adjust the **Phase0** parameter to phase this peak, then adjust the **Phase1** parameter as necessary. Click **OK** when you are finished.

Now that you have a rough idea of the apodization and phase correction parameters, you can proceed with processing the D1(t2) dimension of the 2D data set.

7. Process the D1 (t2) dimension of the 2D data set

Select the **Process/2D Data Processing** menu item. In the first control panel, select the previous ***.ser*** file. In the next control panel, leave the header parameters at their default values (read from the spectrometer header files). They should look like these:

D1 Data Size	**512**
D1 Spectrometer Frequency	**600.1408**
D1 Sweep Width	**7002.801**
D2 Data Size	**32**
D2 Spectrometer Frequency	**60.8**
D2 Sweep Width	**3000**
Source	**Bruker**

Click **OK**.

In the next control panel set the following parameter values:

Data Type	**Complex**
Acquisition in D2	**Echo/Anti-Echo**

Click **OK**.

In the next control panel, set the following parameter values:

Dimension To Process	**D1 FT**
Output Matrix Filename	**bruker.mat**
Dimension 1 Size	**1024**
Dimension 2 Size	**128**
Correct DC-offset	**off**
Correct 1st-point	**none**
Solvent Suppression	**none**
Window Function	**Sinebell^2**
FT Type	**Complex**
Phasing Mode	**Use Parameters**
Phase0	**-84.0**
Phase1	**0.0**
Baseline Correction	**none**
Reverse Vector	**off**
Extract Half Spectrum	**Left Half**
Output Level	**Verbose**
Display Matrix	**on**

Click **OK**.

When the **Sinebell Parameters** control panel appears, enter these values:

Data Size (Points)	**512**
Phase Shift (Degrees)	**90.0**

Click **OK**

There is a slight delay as the `bruker.mat` *matrix is built. FELIX opens the* `bruker.mat` *matrix.*

Click **OK** again to start the D1 transform.

As the D1 transform proceeds, the current row numbers are shown in the text window. This step should less than 1 second.

After the first dimension is processed, FELIX shows the control panel for processing the second dimension.

8. Process the D2 (t1) dimension

Set the following parameter values in the control panel:

Dimension To Process	**D2 FT**
Load Matrix in memory	**off**
Processing Mode	**bundle**
Correct 1st-point	**none**
Solvent Suppression	**none**
Window Function	**Sinebell^2**
FT Type	**Complex**
Phasing Mode	**Use Parameters**
Phase0	**0.0**
Phase1	**0.0**
Baseline Correction	**none**
Reverse Vector	**off**
Extract Half Spectrum	**Left Half**
Output Level	**Verbose**
Display Matrix	**on**

Click **OK**.

In the **Linear Prediction** control panel, set these parameters:

First Point	**1**
Last Point	**32**
Start Point	**33**
End Point	**98**
Number of Coefficients	**8**
Method	**Foward-Backward**

Click **OK**.

In the **Sinebell Parameters** control panel , set these parameters:

Data Size (Points)	**98**
Phase Shift (Degrees)	**90.0**

Click **OK**

Click **OK** to start the D2 transform.

This step should take only a few seconds.

When processing completes, the matrix is open because you chose to display the matrix at completion. The contour threshold is calculated, and the matrix is then displayed.

9. Display the 2D matrix

FELIX calculates the plot levels. You can change them manually:

Select the **Preference/Plot Parameters** menu item. Set the following values:

Contour Threshold	**0.01**
Cor Scheme	**Fire Ramp**

Leave the other values set at their defaults and click Set.

Select the **View/Plottype/Intensity** menu item.

The full 2D spectrum appears.

FELIX always reads data from the matrix, not from a graphics file, so that it can recalculate display parameters at any time. Hence, FELIX redraws the graph with each plot command.

At this point you could examine the D1 and D2 vectors in more detail to determine if further baseline correction or phasing adjustments are necessary.

10. Reference the matrix

Referencing of the matrix happens automatically, since the header parameters are read or adjusted during processing. You can further adjust the referencing, for example, by giving more descriptive names for the axis.

Select the **Preference/Reference** menu item. In the control panel, leave every parameter at its current value, except for these:

Spectrometry Frequency D1	**600.14**
Spectrometry Frequency D2	**60.8**
Axis TextD1	**D1_HN**
Axis TextD2	**D2_N15**

Click **OK**.

The 2D spectrum should now be redisplayed with the correct referencing for each axis.

11. View an expanded-region contour plot

You can choose expanded regions with the cursor or by inputting numeric parameters:

Select the **View/Limits/Set Limits** menu item. When your mouse is positioned over the spectral window, FELIX changes the cursor into a white crosshair cursor.

Holding down the mouse button, drag a box around the region that you want to expand.

When you release the mouse button, the region selected expands to fill the window. The plot is still in intensity mode, hence the contour levels are not shown.

Select the **View/Limits/Manual Limits** menu item.

In the control panel that FELIX displays, the parameters are filled in with the values of the current plot.

Select the **Preference/Reference** menu item. In the control panel, leave every parameter at its current value, except for these:

D1_HN lower	**7**
D2_N15 upper	**9**
D2_N15 lower	**104**
D2_N15 upper	**141**
Limit Type	**ppm**

Click **OK**.

The new 2D region appears.

You can save these parameters and reuse them for other plots. For example, if you were analyzing a series of spectra collected with different mixing times and always wanted to observe identical regions.

Select the **View/Plottype/Contour** menu item to redraw the region as a contour plot.

The 2D matrix is now plotted in contour mode, with individual contours colored as defined by your preference. Use the ***Preference/Plot Parameters*** *command to change your display, as needed.*

12. Change the 2D drawing parameters

If no peaks are visible, try decreasing the contour level to cut lower into the spectrum. If the peaks are outlined but you do not see the circles shrinking to define the tops of the resonances (see Figure 1 on page 37), try increasing the level multiplier to increase the space between levels:

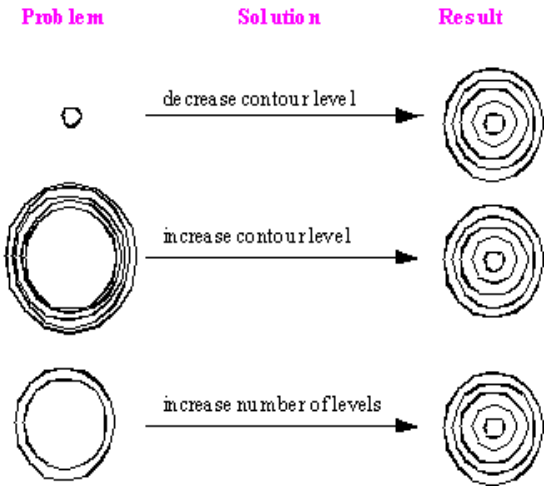

Figure 1 Troubleshooting contour plots

13. Show the grid display

To see the spectrum displayed with an evenly-spaced grid:

Select the **Preference/Plot Parameters** menu item. Click **Axis**. Set **Grid Spacing** to **3** and click **OK**.

Select the **Preference/Plot Parameters** menu item. Click **Axis** and then set **Grid Spacing** back to **0** and click **OK**.

14. Pick peaks

First you need to set the peak-picking parameters. Select the **Peaks/Pick Region** menu item. Leave the parameters at their default values, but set the **Pick Region Mode** to **Define by Cursor**. Click **OK**.

Hold down the mouse button to use the cursor to drag out a box that includes the entire set of desired peaks.

Select the **View/Limits/Manual Limits** menu item.

FELIX displays red boxes around all cross peaks meeting the criteria defined in the control panel. After the peak picking is done, FELIX displays a spreadsheet, displaying all the peaks.

15. Delete and replace peaks

Select the **Peaks/Remove One** menu item. The cursor becomes a **+**. Click one or two red boxes to remove them, then click <Esc> to return to a normal cursor.

Select the **Peaks/Remove Region** menu item. Drag a box around a few peaks to be deleted.

Select the **Peaks/Pick Region** menu item and repeat the dragging to add another region of peaks.

Select the **Peaks/Pick One** menu item and click to add individual peaks. Press <Esc> to return to a normal cursor.

Select the **Peaks/Edit** menu item to manually adjust the box defining a peak. Click the center of any red box of a picked peak. The box becomes green.

Click the center of the box and drag to move the entire box or click near a corner of the box and drag to resize it.

To leave editing mode, press the <Esc> key.

Select the **View/Plot** menu item to redraw the window (and clean up any broken lines or other details).

16. Assign the cross peaks

Select the **Peaks/Name One Peak** menu item and click one of the red boxes.Set the following parameters to assign the resonance:

Item Number	**148***
D1 peak namer	**h1**
D2 peak name	**null**

**Example integer only. The number in your display should match the number of the peak you select.*

Click **OK**, then press the <Esc> key to return to a normal cursor.

You do not need to assign the peak in both dimensions. You can label the cross peaks in one dimension at a time, as the assignment is made. This is usually how assignments are observed.

If you want to use the restraints list directly in the Insight II or Discover program, you have to use the Insight II proton names as the peak names. At the moment there is no check of atom names, so you may enter anything you want.

17. Display assignments

Select the **Peaks/Find** menu item, select **Find Peak By Name** and set the **Action** to **Color**. Set the **Peak Name D1** to **h1** and **Peak Name D2** to *****. Select **Yellow** for **Color**. Click **OK**.

*FELIX searches the assignment list, and colors the boxes surrounding all peaks with a label of **h1** in **D1** dimension yellow.*

18. Calculate volumes

To calculate the volumes of the picked peaks, select the **Measure/Integral/Volume** menu item. In the control panel, select the **Measure All Volume** option for **Action**.

In the next control panel, leave the **Peak** and **Volume** set at their defaults. Set **Volume Slot Number** to **1** and **Mixing Time** to **0.1**. Click **OK**.

FELIX displays a **Building New Volume Entity** control panel. Set **Total Mixing Time Slots** to **6** and click **OK**.

You can now view the volume data with the **Edit/Table** menu item (selecting the ***vol:volumes*** table) or write the volume data to a file with the **File/Export/Table** menu item.

To calculate restraints from these volumes based on the two-spin approximation, you must open or create a scalar entity for the database, define a scalar pair, create the restraints (strong–medium–weak, or any other listed choice), and write the restraints file. The appropriate commands are in the ***Measure*** *menu.*

19. Quit FELIX

To quit FELIX, select the **File/Exit** menu item.

Writing your own macros

FELIX macros are the most powerful and innovative feature of this NMR processing software. By writing your own macros, you can automate anything that you can do with FELIX manually. Your ability to transform and manipulate data automatically using macros is limited only by your imagination.

FELIX 2002 comes with a library of macros capable of many common processing tasks. You can modify these macros to fit your specific needs.

Note

In addition to using macros for custom data-processing and data-analysis tasks, macros also define the parameters of the FELIX graphical interface. In fact, the advanced user may use macros to create control panels and menus in order to design a custom environment.

Chapter 4, “Macros” of the FELIX *Command Language Reference* provides much more information about writing macros. Its Appendix C, “Example Macros” provides many illustrations of macros and how to use them in FELIX. The two examples below are from this Appendix.

To write or edit a macro, it is easiest to use your system text editor. Any editor may be used as long as the resultant files *do not* contain formatting characters and *do* contain standard carriage control.

It is standard for the first line of any macro to contain the macro’s name. However, this is optional.

FELIX ignores any macro line that starts with c**. The beginning of a typical macro is shown below.

Caution

The line numbers at left are used for reference only, and should ***not*** be included in the macro.

```
1    c**users.mac
2        set 0
3        dr
4        ...
```

Macros may also contain tab characters and blank lines, so that they may be organized to enhance readability. In addition, any characters that follow a semicolon (;) are ignored by the macro interpreter. This makes it easy to add comments to macros, as shown below in Lines 2, 4, and 17:

```
1    c**users.mac
2 ; Close all graphics frames:
3    fra zero
4 ; Open first graphics frame with a size of 100x100 pixels
5    fra open 10 10 100 100
6 ; Resize the frame to a size of 500x400 pixels
7    fra resize 10 10 500 400
8 ;
9 ; Open another frame with a size of 600x500 pixels
10   fra open 30 30 600 500
11 ; Set the first frame as the current frame:
12   fra front 1
13 ;
14   set 1 ;set all the points in work space to 1
15 ; performs a sinebell multiplication (size=all points,shift=90)
16   sb &datsiz 90
17   dr       ;draw the sinebell window
18 ;
19   ret      ;return to GUI or the caller macro
20   end
```

Please refer to the FELIX *Command Language Reference* for more in-depth guidance on writing FELIX macros. Online, find the FELIX 2002 documentation at this URL address:

http://www.accelrys.com/doc/life/index.html

Navigate to the FELIX 2002 documentation. Look for Appendix C, “Macros”; here you can view and print the file.

Note

If you are prompted for a username and password at the Accelrys documentation website, use the following:

Username: **science**

Password: **faster**

Sample Macros

Example 1: eval_point.mac

```
; Macro evaluates a particular point in each
; vector of a serial 2D data file and stores
; output in a FELIX macro file. Macro presents
; example of using one macro to build another
; macro.
;
     get 'Input Data File -->' inpdata
     get 'Output Data File -->' outdata
     get 'Data Point to Measure -->' point
     get 'Number of Exps -->' num_exp
     opn txt &outdata 0
     for loop 1 &num_exp
             re &inpdata
             gv &point dataval
             put &dataval
     next
     cls
     end
```

.

Example 2:
lpf_d2.mac

```
; Simple macro to adjust the 1st point in a
; D2(t1)-vector of a transformed 2D matrix
; using LP. Removes missampling artifact in
; virtual acquisition. Caution, original
; matrix is overwritten.
;
     get 'Specify matrix -->' mat
     inq mat &mat exist
     if &exist eq 0 then
              ty Matrix &mat not found!!!
              go scram
     eif
;
     cmx
     mat &mat w
;
     for row 1 &d1size
              loa &row 0
              hft

              ift
              lpf
              ft
              mul 2
              red
              sto &row 0
              ty row=&row
     next
 scram:
     ret
     end
```

Using the FELIX database and spreadsheets

Introduction to the database utilities

In this lesson you will learn about the commands and functionalities of the database commands in FELIX.

1. Start FELIX

Start FELIX by double clicking the **Felix** icon on your desktop, or by clicking **Start** on the Windows taskbar, then selecting **Programs/Accelrys Felix 2002/Felix 2002**.

If FELIX prompts you to restore from last session, click **Cancel**.

The FELIX main window appears with an empty graphics frame, Frame 1.

FELIX displays the **OPEN DATABASE FILE** dialog box. Navigate to your working folder; then, type in a new filename (e.g., ***dba0***) to open a new empty database.

The name of the database file (as well as the directory of the file) is displayed in the title bar of the FELIX main window, confirming its selection

The FELIX database has a hierarchical structure, illustrated in Figure 2.

Files are composed of entities or tables whose structures are defined by schema files. The entities are in turn composed of items, which are themselves an arrangement of elements. The dba file system is difficult to understand in an overall sense, but one can begin to become familiar with it by working through some of the dba utilities, as in this lesson.

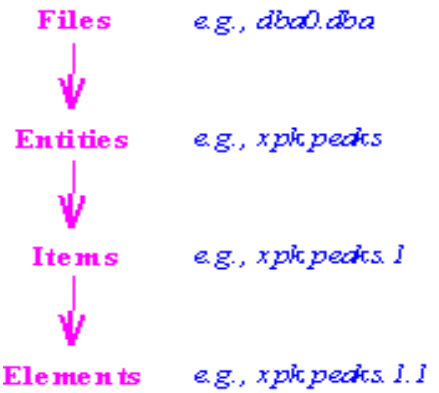

Figure 2 FELIX database hierarchical structure

2. Close the current dba file and create a new one

Click inside the command text field at the bottom of the FELIX window. Enter the following commands (press <Enter> after typing each command), which closes the current dba file, creates a new one, opens it, and then lists the entities in the new dba file:

> **dba file close quit**

> **dba file build test** (*if you already have a dba file named test, use some other name*)

> **dba file open test**

> **dba file show**

You should now see the following in the text window:

```
item page name schema
---- ---- ---- ------
1      1      dba    dba
```

which indicates that only the default (empty) database file exists.

Note

FELIX remembers up to 10 used commands. You can use the up or down arrow keys to browse through the last commands and edit one of them.

3. Generate 2D cross peaks

Select **File/Open**, set **File Type** to **Matrix** (*.mat) and open any 2D spectrum (e.g., the one created in "Processing a 2D spectrum" on page 28). Select **Peaks/ Pick Region** to pick a small region of peaks.

*The **Peaks/Pick Region** command knows how to render the data, even without your specifying a schema explicitly. This is because it knows which entity it requires and automatically uses the appropriate one (i.e., xpk.sch).*

4. Check the database file structure and see how it has changed

Select **File/Open**, set **File Type** to **Matrix** (*.mat) and open any 2D spectrum (e.g., the one created in "Processing a 2D spectrum" on page 28). Select **Peaks/Pick Region** to pick a small region of peaks.

You should now see the following in the text window:

```
item page name schema
---- ----- ---- ------
1           1      dba    dba
2           3      xpk    dba
```

5. View the contents of the entity xpk

Now enter:

```
> dba entity show xpk
```

You should see this in the text window:

```
item page name schema
```

```
---- ----- ---- ------
1    5      peaks xpk
```

6. Inquire about particular items and elements of the entity xpk:peaks

Enter:

```
> dba entity show xpk:peaks
```

*FELIX displays a list of the cross peak footprints determined by the **Pick** utility. Until displayed, you can also view a table of the peaks' contents by using the **Edit/Peaks** menu item. This creates a special table that contains information about the peaks. You can use this table to edit the items or cells of the entity.*

You can also specify the display of a particular item in an entity.

Enter:

```
> dba item show xpk:peaks.2
```

Information similar to this appears in the text window:

```
2 216.186 2.383 0 null 721.749 3.269 0 null
```

Next you specify a particular element in an item.

Enter:

```
> dba element show xpk:peaks.2.2
```

Information similar to this appears in the text window:

```
216.186
```

Since the element fields are named, you can use an equivalent command:

Enter:

```
> dba element show xpk:peaks.2.cen1
```

The same information is displayed as for the preceding command:

```
216.186
```

The other database utilities have the same syntactic logic.

7. Load the value of an element

Now you load a value from the database using the name check.

Enter these commands:

```
> dba element load xpk:peaks.2.cen1 check

> lis check
```

The following value is displayed:

```
216.186
```

You can change the value of any element in the database using an identifying number.

Enter:

```
> dba element store xpk:peaks.2.cen1 104.8
```

You can also change the value of any element in the database by using names instead of numbers.

Enter these commands:

```
> def check 104.8

> dba element store xpk:peaks.2.cen1 &check
```

8. Modify schema

You begin by copying one of the existing schema, asg.sch, to a new schema with the name wrd.sch. Then you edit this new schema file.

Note

To locate the FELIX schema files, locate the **database** folder in the path where the FELIX 2002 executable is located.

By default this path is:
C:\Program Files\Accelrys\Felix 2002\database.

Open the **database** folder. Locate and open the folder called **schema**. Find the schema file you need.

Copy the existing schema, ***asg.sch***, to a new file named ***wrd.sch*** in your working directory using Windows Explorer. Next use Notepad to edit the new ***wrd.sch*** schema file to the following:

```
c**wrd.sch
wrd 5
item       i k     01      06      (1x,i5)
cenpnt     r k     01      10      (f10.3)
wid        r       01      10      (f10.3)
cenppm     r k     01      10      (f10.3)
name       c       32      34      (2x,a32)
```

Note that three numbers need to be changed in the last line.

The working directory is the folder where you created the database file. You can check or modify this by selecting ***Preference/Directory***

9. Pass data to and get data from a new database entity

Generate a new entity by entering this command:

```
> dba entity build weird wrd 1
```

This generates a new entity with the name weird, which is based upon the schema ***wrd.sch****, using a single occurrence of that schema.*

Store a value in an element of your new entity by entering:

```
> dba element store weird.1.5 abcdef
```

Equivalently, you could also enter:

```
> dba element store weird.1.name abcdef
```

Both commands specify storing the string in the entity named weird, item 1, element 5 (again note that the element fields are named).

Give that element a name by entering:

```
> dba element load weird.1.name var
```

Confirm that the element has been named by entering:

```
> lis var
```

You should see the following:

```
abcdef
```

Write the entity to an ASCII file by entering:

```
> dba entity write weird weird.txt
```

Now read the ASCII file back in as another entity by entering:

```
> dba entity read test weird.txt
```

Confirm the success of this set of operations by entering:

```
> dba element load test.1.5 newvar
```

```
> lis newvar
```

The following should be displayed:

```
abcdef
```

*To view any entity via tables you can use the **Edit/Table** menu item. This opens a control panel from which you can choose the entity that you would like to display in a table.*

Closing files and exiting FELIX

To exit FELIX and return to your operating system, select the **File/ Exit** menu item.

If changes have been made to the FELIX database (which contains spectrum information such as cross peaks, baseline points, etc.), FELIX displays a dialog box prompting you to save changes before exiting.

6. Getting More Help

More help for FELIX 2002 is online. To access it, visit the Accelrys website:

http://www.accelrys.com/doc/life/index.html

Accelrys posts updates or corrections to the web site, assuring this information is the most current. FELIX 2002 documentation is found in the **Life Science Documentation** section.

Note

If you are prompted for a username and password at the Accelrys documentation website, use the following:

Username: **science**

Password: **faster**

Although these online documents include indices and tables of contents, you can also use the Accelrys Site Search at:

http://www.accelrys.com/search.html

Select **All Documentation** in the **Search Area** list. Enter term(s) in the **Search** field, then click **Search**.

While viewing the document online, you can use the searching capabilities of your browser to locate information.

You can print individual chapters of these documents via your browser's printing capability.

The FELIX help available online includes the documents described below.

FELIX User Guide

The FELIX User Guide gives a more complete review of how to work with *FELIX*. The topics include:

- Working with the interface.
- Theory of NMR processing.
- Theory of resonance assignment
- Theory of analysis of protein-ligand interaction spectra
- 1D, 2D, and ND processing of NMR data.
- Use of the Assign module
- Use of the Autoscreen module
- Hot-key reference.
- File formats.
- FELIX startup.
- Data transfer and conversion.
- The *FELIX User Guide* also contains several appendices. These provide additional information that might make installing and running FELIX easier.
- Appendix A, *References*, contains complete references for citations made in the text.
- Appendix B, *Keyboard Shortcuts and Accelerator Keys*, lists keyboard shortcuts for the commands in the interface.
- Appendix C, *Felix Startup*, gives helpful hints on starting FELIX the first time.
- Appendix D, *Data Files*, list important file formats.

FELIX Tutorials

The FELIX Tutorials provide step-by-step procedures illustrating typical examples of processing raw NMR data, use of the database, use of the Assign and Autoscreen modules. These lessons address a range of NMR data processing and analysis topics.

FELIX Command Language Reference

The *Command Language Reference* is a complete guide to FCL, the command language underlying the FELIX program. It provides information about the basics of FCL, symbols and expressions, macros, real-time displays, menus (and how to customize them), the database, and commands. Appendix C contains some useful example macros.

The *FCL Command Language Reference* is intended for advanced FELIX users who want to modify the user interface, write macros, and do other operations that require FCL.

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7. Keyboard Shortcuts and Accelerator Keys

Keyboard shortcuts

Most FELIX 2002 menu items have keyboard shortcuts. Use these when you prefer not to access menu items with the mouse.

1. First, access the dropdown menu by pressing the <Alt> key, and then pressing a key as the underscored letter in the menu name you want to access.
2. Next, select a menu item from the dropdown menu by pressing the hot key again as the underscored letter in the item name. For example, press <Alt>+f> for the **File** menu.
3. Then, in the example, press o to access the **Open** item. (In FELIX documentations, this is abbreviated, as in <Alt>+fo.)

Since the shortcut keys are very obvious from the menu names, they are not listed in this chapter.

Note

> Usually, the underscores in the menu names (for example, **O**) are not visible until you press the <Alt> key.

Accelerator keys

Some menu items have accelerators (usually the <Ctrl> key and a letter, as listed below). These items do not require you to go through the menu hierarchy to access the item or perform the action. Just press the accelerator keys to directly access the menu item. For example, **<Ctrl>+o** to open a file.

Access these accelerator keys by pressing the <Ctrl> key and the other letter simultaneously. They are visible in the menus (after the corresponding menu items).

Command	Keystroke
<Ctrl+o>	File/Open
<Ctrl+p>	View/Plot
<Ctrl+1>	View/Plottype/1D
<Ctrl+i>	View/Plottype/Intensity
<Ctrl+c>	View/Plottype/Contour
<Ctrl+s>	View/Limits/Set Limits
<Ctrl+f>	View/Limits/Full Limits
<Ctrl+k>	View/Draw Peaks
<Ctrl+l>	Peak/List

Pulldown-independent functions

You can access some accelerator keys using a single keystroke, as described in the tables below. These do not require you to press the <Alt> or the <Ctrl> key.

Note

To use the number pad on your keyboard to execute these functions, you must toggle the <Num Lock> key to **on.**

Command	Keystroke
Pan left and down	1
Pan down	2
Pan right and down	3
Pan left	4
Grab and drag	5
Pan right	6
Pan left and up	7
Pan up	8
Pan right and up	9
Step one plane up *(3rd dimension in 3D or 4D)*	<up arrow>
Step one plane down *(3rd dimension in 3D or 4D)*	<down arrow>
Step one plane up *(4th dimension in 4D)*	<right arrow>
Step one plane down *(4th dimension in 4D)*	<left arrow>
Select new plane *(if frame connection is on and the primary frame is the active frame)*	.
Zoom in *(half limits)*	-
Zoom out *(double limits)*	–

If the active display is a 1D slice

Command	Keystroke
Pan left	4
Pan right	6
increase intensity	8
decrease intensity	2
half limits	-
double limits	–

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8. Contacting Accelrys Support

If you have questions about FELIX 2002 that are not answered here or in the FELIX online documentation at:

http://www.accelrys.com/doc/life/index.html

please contact Accelrys support for your area.

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