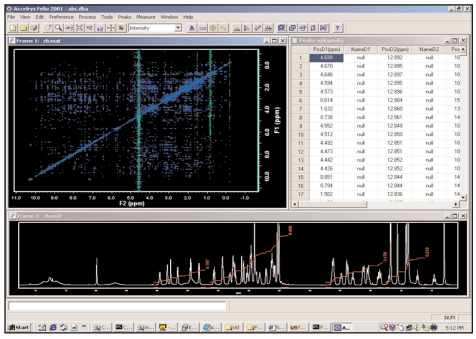
Quickly transform raw data to spectra

The industry standard software for off-line NMR data processing, spectral visualization, and analysis

Automatic and semi-automatic NMR spectral assignment

FELIX

Raw data collected from a modern NMR spectrometer needs to be converted into a form that enables extraction and interpretation of structural and dynamical information about the system under investigation. The first step involves the transformation of time-domain data to the frequency domain using mathematical algorithms, such as apodization, Fourier transformation and linear prediction. The next step is the extraction of the spectral features, such as peak positions, peak integrals, peak line widths and peak separations. The numerical values extracted from the spectra are then analyzed in light of known physical models and converted into geometric restraints. The strong data processing and spectral analysis capabilities found within FELIX allow the spectroscopist to transform raw data, and begin the process of structure and dynamics determination based on NMR.



The graphical user interface of FELIX allows for streamlined processing and analysis of your NMR data.

FELIX Products

FELIX is available in server-side or desktop versions.

- *FELIX*: for SGI IRIX or Red Hat Linux; modules available include FELIX 2D, FELIX ND, FELIX Assign, FELIX Analytical, FELIX Autoscreen, and FELIX Model
- *FELIX Desktop*: for Windows PCs; modules available include FELIX 2D, FELIX ND, FELIX Assign, and FELIX Autoscreen

FELIX 2D and FELIX ND

FELIX is the industry standard software program for off-line data processing, spectral visualization, and analysis of all types of high resolution, 1D to 4D homonuclear, and heteronuclear NMR data. FELIX is built upon the foundations of a relational database, an extensive macro language, and an easy-to-use, multi-windowed, menu-driven interface, which allows for quick and easy performance of routine tasks. FELIX comes equipped with dozens of built-in and tested data processing macros, and has the ability to directly read data from all of the major spectrometers from Bruker, Varian, and JEOL. Along with an unsurpassed range of algorithms for processing data and a powerful macro language, FELIX gives you the freedom to choose how to process your data and create novel solutions for your most sophisticated NMR data processing needs.

Highlights

- User interface with icon driven functions to provide streamlined access to commonly used functions
- Flexible visualization of spectra including:
  - visualization and correlation of multiple spectra
  - tile and strip plots for viewing multi-dimensional spectra
  - canvas mode which allows you to expand spectra to sizes larger than your monitor
- 'E-Z' macros that allow you to quickly process all spectra from one to four dimensions including:
  - States-TPPI spectra
  - Echo-anti-echo N/P gradient type data
  - Oversampled Bruker digital data
- 'E-Z' macros that allow you to flexibly incorporate a range of processing features including:
  - Solvent suppression
  - Interactive phase correction
  - Hilbert transforms
  - Linear prediction (all methods)
  - Fourier Transforms
  - Interactive base-line corrections
  - Flexibility to customize all your macros
- Robust and accurate peak picking algorithms that are crucial to automated assignment protocols
- Spreadsheet like tables that allow you to easily visualize and edit the results of peak picking and other spectral information
- Several choices of baseline correction[1], solvent suppression, and peak picking algorithms
- Relaxation analysis feature to help you easily extract dynamic information
- Ability to overlay planes from different matrices (FELIX ND)*

FELIX Assign

FELIX Assign provides automatic and semi-automatic capabilities for NMR spectral assignment of biological macromolecules, encompassing all the stages of spin system detection, spin system identification, resonance and cross-peak assignment, and restraint generation. A broad range of spectra can be analyzed, from homonuclear 2D spectra to

* Features new to FELIX 2004 are marked with an asterisk.

heteronuclear double- and triple-resonance, 3D and 4D spectra using methods developed in collaboration with Dr. R. Kaptein (Utrecht, Netherlands)[2] and Dr. D. Marion (Grenoble, France)[3]. The sophisticated algorithms (such as those based on fuzzy algebra and global optimization for spin system identification and sequential assignments, as well as the great variety of manual tools for generating overlaid spectra, correlated frames, tiles, and strip plots) make FELIX Assign invaluable during the complex task of spin system assignment. FELIX Assign can literally save years of effort by tracking, managing, and automating the assignment process.

Highlights

- Spin system detection and sequential assignment for numerous experiments:

  2D & 3D Homonuclear
  - 2D COSY/TOCSY/NOESY
  - 3D TOCSY-TOCSY/TOCSY-NOESY/NOESY-NOESY

  2D & 3D Double Resonance
  - 2D 15N HSQC
  - 3D 15N HSQC-TOCSY
  - 3D HCCH-TOCSY

  3D Triple Resonance
  - HNCO/HNCA/HN(CO)CA
  - CBCANH/CBCA(CO)NH
  - HNCO/CBCANH/CBCACO(N)H
  - HNHA/HNCACB/CBCA(CO)NH

  4D Triple Resonance
  - HNCAHA/HN(CO)CAHA

- Ability for user to define assignment protocol if alternative experiments performed
- Flexible overlay of spectra
- Automated and manual NOE crosspeak assignment for:
  - 2D NOESY
  - 3D NOESY-NOESY
  - 3D and 4D heteronuclear edited NOESY spectra
- Generation of restraints that can be read by Insight II's NMR Refine DGII, NMR Refine Advanced, NMR X-PLOR, and CNX-NMR

Felix Analytical

FELIX Analytical provides chemists assistance in resonance assignment of small molecules including structure display and labeling. A broad range of spectra can be analyzed for homo and heteronuclear 2D methods including:

- COSY, TOCSY
- HMQC & COSY
- HMQC & TOCSY
- HMQC & COSY & TOCSY
- HMQC & COSY & HMBC
- HMQC & TOCSY & HMBC

FELIX Autoscreen

FELIX Autoscreen supplies the tools necessary for effortless processing and management of large sets of NMR data. An unlimited number of spectra can be handled through the use of its project database. In addition, automated peak matching and scoring algorithms offer a quick and easy way to analyze specified data sets and compare scoring contributions. FELIX Autoscreen can also cluster experiments with commonly displaced peaks to help identify individual binding sites in a protein. Additionally, with FELIX Autoscreen you can mark unmatched control peaks by crosses, and unmatched test peaks by diamonds to graphically visualize unmatched peaks.*

FELIX Model

FELIX Model provides direct interaction between experimental 2D-NOESY spectra, molecular structures, and back-calculated 2D-NOESY spectra within a single integrated interface. FELIX Model allows you to judge the accuracy of a given model, and suggest potential new cross-peak assignments where crosspeaks have been erroneously assigned. The novel features available within FELIX Model allow you to simultaneously view and interact with molecular data in Insight II and spectra in FELIX, which will help you develop a detailed understanding of how your experimental NMR data defines actual structural features.

System Requirements

- SGI: IRIX 6.5.19-6.5.24 on R10000 and higher
- Linux: Red Hat Enterprise Linux WS 2.1 and WS 3.0 on Intel Pentium III and higher (32-bit support only)*
- Linux Graphics: NVidia Quadro4 980 XGL and Quadro4 FX1100 graphics cards using appropriate drivers from NVidia
- Windows: Windows 2000 SP3 and SP4, XP SP1 and SP2 on Intel Pentium III and higher (32-bit support only)

Complementary Software

- NMR Refine DGII, NMR Refine Advanced, and NMR X-PLOR (Insight II modules available on SGI, not Linux)
- CNX-NMR

References

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4. Blake, P. R., Park, J. B., Bryant, F.O., Aono, S., Magnusen, J. K., Eccleston, E., Howard, J. B., Summers, M. F., and Adams, M. W. W., *Biochemistry*, **1991**, 30, 10885.
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accelrys®

Accelrys Corporate Headquarters
10188 Telesis Court
San Diego, CA 92121, USA
Tel: +1 858 799 5000

Accelrys European Headquarters
334 Cambridge Science Park
Cambridge, CB4 OWN, UK
Tel: +44 1223 228500

Accelrys Asia Headquarters
Nishi-shimbashi TS Bldg 11F
Nishi-shimbashi 3-3-1, Minato-ku,
Tokyo, 105-0003, Japan
Tel: +81 3 3578 3860