NAME

nmrWish – Tcl/Tk Window Shell for Spectral Analysis

DESCRIPTION

The **nmrWish** program is a version of the Tcl/Tk window shell **wish**, customized to include facilities for manipulation, display, and analysis of multidimensional spectra and images. It is a companion to the NMRPipe System, the spectral processing system based on UNIX pipes (Delaglio et al., 1995).

Tcl/Tk is a powerful and widely used command language which includes facilities for graphical interface creation and for communication between different applications; it was introduced to the NMR community in the package **NMRView** (Johnson and Blevins, 1994). The originator of Tcl/Tk, John Ousterhaut, developed it initially to provide an extensible command language for engineering applications (Ousterhaut, 1994).

A key feature of Tcl/Tk is the ability to construct a complete graphical user interface as a simple script, rather than as a lengthy compiled program. Because of its power and convenience, Tcl/Tk has found use in thousands of scientific and commercial applications, including those of NMR spectrometer manufacturers and molecular modeling software companies.

As a scripting language, Tcl includes facilities for manipulating variables, text patterns, and lists, and for evaluating numerical expressions. It also provides basic text file input/output, looping and conditional statements, and for the definition of procedures. A special feature of Tcl is the *associative array*, an array whose index is an arbitrary text string rather than an integer, and whose contents may be a combination of numeric or text data.

As a graphical interface language, Tk includes facilities for creating various types of buttons and menus, as well as items such as scrollbars and text editing windows. It also includes facilities for rendering simple graphical items such as polygons, ovals, and text. All of the graphical items support many modes of interaction, so that interfaces with options such as real−time drag−and−drop can be created.

In addition to the usual features of Tcl/Tk, the special facilities of NMRWish include the following:

Region Extraction: Extraction or projection of arbitrary spectral Regions of Interest (ROIs). Extracted regions can be centered or aligned automatically through interpolation, so that the extracted data corresponds to the requested chemical shift coordinates regardless of the digitization of the data. Furthermore, extracted regions which exceed the measured chemical shift window are unfolded and sign-adjusted automatically, so that regions from related spectra can be manipulated or displayed consistently even if they have differing spectral windows.

Graphics of Spectra and Images: PostScript output with completely customizable page layout is provided. Hard copy of 1D spectra and 2D contours are available, as well as hard copy modes for single images, three−image RGB composites, and image vs. image scatter plots. More recently, facilities for screen−based multi−window spectral and image graphics have also been included.

Peak Detection: automated peak detection in 1D-4D, including options for identifying peaks due to random noise and truncation artifacts.

Relational Database Engine: a simple, general purpose database engine, capable of manipulating peak tables, assignments, and PDB format molecular coordinates.

Binary Manipulation: general facilities for reading, writing, and manipulating binary data, including type conversion (e.g. integer to float) general−purpose vector processing commands and access to NMRPipe processing functions. Specific commands for manipulating and interpreting

NMRPipe−format data headers are also included.

Illustrations of nmrWish applications include spectral format conversion, custom hard−copy format design, peak picking and peak evolution extraction, multi-spectrum visualization and triple-resonance backbone assignment, automated generation of NOE constraints, and tools for SAR by NMR (Fessik et al., 1996).

LEGAL NOTICES

The **nmrWish** program and its related software is based on a design originating in the NIH Laboratory of Chemical Physics, NIDDK. It is not to be distributed or modified. (C) F. Delaglio 1997.

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The **nmrWish** program makes use of GIF format images. The Graphics Interchange Format(c) is the Copyright property of CompuServe Incorporated. GIF(sm) is a Service Mark property of CompuServe Incorporated.

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