Stand-Alone NMR Data Processing

MacFID
Tecmag
6006 Bellaire Blvd.
Houston, TX 77081
713-667-8747; 713-667-3180 (fax)
Version 5.0; $950

MacFID 2D is a powerful, well-documented program for processing, displaying, and archiving routine 1D and multidimensional NMR spectra. It was developed by Tecmag, best known for upgrade packages for aging NMR spectrometers. A typical upgrade involves replacing the original data system and pulse programmer with a Tecmag hardware unit and a Mac loaded with *MacNMR 5.1* to run all tasks controlled by the original data system.

MacFID is essentially *MacNMR* without the ability to control the spectrometer hardware. Tecmag has upgraded more than 100 spectrometers, and a number of laboratory-built spectrometers and magnetic resonance imagers also use Tecmag control units; we have Tecmag controllers on four of our spectrometers. Because Tecmag software is so widely used, the company makes its software as complete as that of the major spectrometer manufacturers.

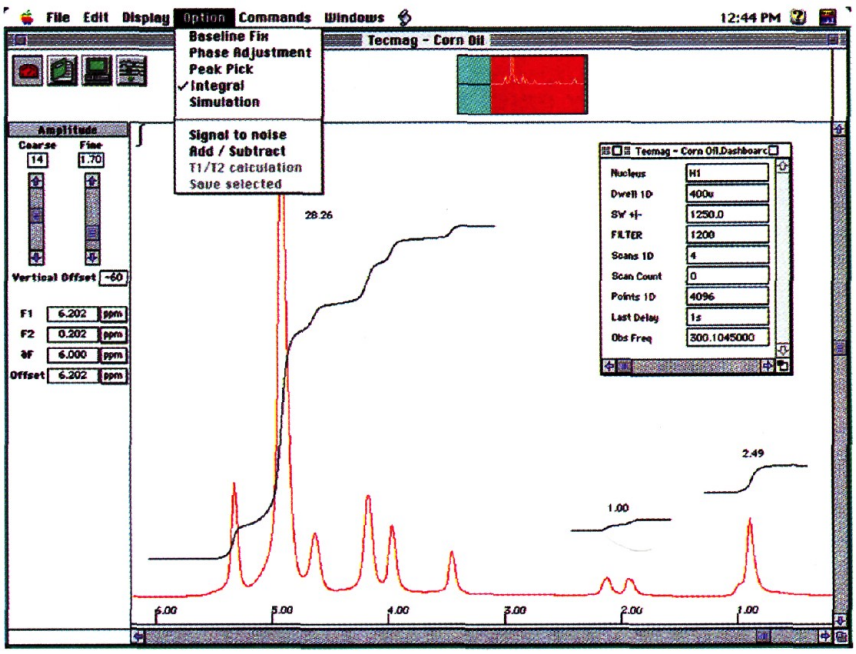
Two versions are available: one for the so-called 68K Macs with math coprocessors and one written in native Power PC code for RISC-based Macs. The hardware requirements suggested are reasonable—16 MB RAM and a 230-MB hard disk. If users primarily process 1D data sets, 16 MB RAM may be more than they need, but the program becomes RAM hungry with large, multidimensional data sets, and a 230-MB hard disk quickly fills up as one processes multidimensional spectra. Copy protection is achieved by a hardware key, but Tecmag distributes copies of software for processing 1D data free. Mac OS System 7.1 or later is required.

We found this version to be stable and close to bug free, and we were unable to crash it. We did not observe any conflicts with other common Mac programs.

As with any software, differences in the personal preferences of the users and programmers can be found. Tecmag's product is as good as the software used by most major spectrometer vendors and better than some. It has standard features you would expect: flexible apodization and baseline correction, integration, line fitting and simulation, spectral addition/subtraction, and some degree of autophasing. Individuals can boot the software via user files, providing custom configurations. The plotting software is more powerful than alternative packages, and it easily provides for exporting color graphics in the common "PICT" format.

The program has some faults, although they tend to be minor. For example, we dislike programming conventions that create unit discrepancies between the data axis and parameter boxes. The zoom feature in contour plot mode is awkward, and we find it difficult to reproducibly zoom on specific regions of 2D spectra.

One powerful feature is the implementation of AppleScript, a Mac OS system extension that allows automation of repetitive and/or complex tasks that transcend typical macroing. Scripts can be written in a programming language or recorded by performing a series of point-and-click operations of arbitrary complexity. The result is an executable program that will reproduce those actions. NMRscripts, Tecmag's name for scripts used with *MacFID*, can be accessed via the script menu in *MacFID*. This allows a high level of customization for specialized data processing tasks. You can create scripts that automatically process NMR data, then manipulate the data or graphics within other applications.



Mac FID's integration and scrollable dashboard windows contain all the imported native parameters.

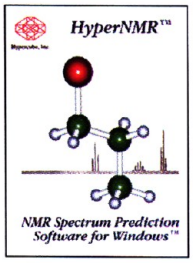
Documentation is generous and helpful. An appendix treats aspects of data transfer and conversion. Data filters for many formats are provided, and they preserve essentially all acquisition parameters in a logical generic format. Comments of up to 1024 characters can be saved. Most data formats not supported with full filters can be read without conversion of acquisition parameters; however, they could be manually re-entered if needed.

MacFID 2D facilitates documentation of experimental work and archival storage. Because most new Macs ship with built-in Ethernet, an NMR lab with a server or redundant mass storage devices and Quadras or PowerMacs running *MacFID 2D* can have a fairly sophisticated way to archive and protect data.

This is the best NMR software we have seen for a personal computer. We suspect that many spectroscopists who might benefit from this software will consider using it regardless of the type of machine on their desk.

Reviewed by James F. Haw and David B. Ferguson, Texas A&M University

Predicting 1D NMR Spectra



HyperNMR
Hypercube
419 Phillip St.
Waterloo, Ontario, Canada N2L 3X2
800-960-1871; 519-725-5193 (fax)
Version 1.0; $995 (commercial); $695 (academic and government)

HyperNMR is intended for a priori predictions of one-dimensional NMR spectra. It can be used in a stand-alone mode if 3D molecular coordinates are available in a *z*-matrix format or in conjunction with Hypercube's *HyperChem* molecular design software. When *HyperChem* is available, the user constructs a molecule in that environment, and the resulting optimized structural information is transferred into *HyperNMR* by dynamic data exchange.

Although the stated minimum requirements for *HyperNMR* are a 386 CPU and a math coprocessor, 4 MB RAM, 4 MB free hard disk space, a VGA display, Windows 3.1, and a mouse, a 486- or Pentium-based machine running at 50 MHz or more and at least 8 MB RAM provides more satisfying performance. Under this preferred configuration, the NMR shielding and coupling constant calculations are performed in reasonable times (seconds to minutes) once the molecular coordinates are transported into *HyperNMR*. The two examples in the tutorials, methane and four protons of a restricted 16-carbon region in a protein, require ~ 15 s and 2 min, respectively, to calculate the corresponding proton spectra.

After spectra are generated, they can be displayed in line format or as Lorentzian or Gaussian resonances at a preselected field strength. In the latter case, the distribution widths can be adjusted by using the mouse and a sliding button on the upper portion of the screen. Similarly, position within the spectrum can be adjusted by using a sliding button in the lower portion of the screen. In terms of data display, the only feature I found somewhat inconvenient was the inability to set the chemical shift limits in the spectrum.

Users even slightly familiar with molecular construction via *HyperChem* or able to retrieve stored information will need only a few hours to complete the tutorials. The general layout of working screen and tool icons is similar to those in *HyperChem*. Spectral calculations can be carried out using TNDO/1 or TNDO/2 semiempirical methods; Slater exponents for shielding and slow three-center integrals can be added. Shielding and spin–spin coupling can be calculated or turned off.

The tutorial manual is easy to follow and provides step-by-step details of *HyperNMR*'s features. It contains six chapters that cover general operations and manipulations, reference information, and scientific background. Chapter 6's organization is textbook quality and provides a nice overview of NMR and the computational aspects of the program, including magnetic shielding, nuclear spin coupling, various semiempirical methods, and perturbation theory.

The weakest part of the manual is that once the tutorials are completed, an individual less familiar with NMR may obtain the false impression that the software is capable of generating proton-coupled ^{13}C spectra as well as proton-decoupled spectra in the natural abundance format. However, only the decoupled spectrum can be obtained.

Because the program does not recognize the natural abundance of an isotope, one must label the various atoms to obtain the carbon spectrum of a molecule. This is easy to do, but it introduces the additional coupling not found under natural abundance conditions. The broadband decoupled ^{13}C spectrum can be obtained by restricting the Fermi spin–spin coupling. This is accomplished in the shielding and coupling options screen. However, there are no features in the program to obtain the proton-coupled natural abundance ^{13}C spectrum because removal of the Fermi spin–spin coupling affects both the carbons and protons.

HyperNMR is a simple and easy-to-use program that is most useful for determining proton spectra for molecules containing elements ranging from hydrogen to argon. In the case of ^{13}C information, it is limited to proton-decoupled calculations. *HyperNMR* also can be used to predict ^{15}N-, ^{19}F-, or ^{31}P-enriched spectra. Although the computed values and resulting spectra for these isotopes are not exact, they are reasonably close to experimentally measured parameters and are useful for structural interpretation.

Reviewed by R. K. Gilpin, Kent State University