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APPLICATION NOTE

WHNMR—A UNIVERSAL NMR APPLICATION PACKAGE

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Abstract—A PC-based NMR off-line data processing system is developed and described in detail. With this software system, one-dimensional (1D), two-dimensional (2D), and NMR imaging (MRI) data can be processed easily, and give reliable results. By the applications of this system, a versatile software interface is set up to achieve data exchanging and integrated usage with other PC application software and aids the PC to become an effective and powerful workstation.

INTRODUCTION

With the advance of Fourier Transform (FT) Nuclear magnetic resonance (NMR) spectroscopy in technique and application, more and more NMR data have to be processed and analyzed in practical applications, exploiting a large amount of dedicated computer time of the spectrometer. In this case, some off-line NMR data processing application systems appear naturally. With the rapid progress in computer technology, the current generation of the NMR spectrometer is equipped with excellent data processing and application packages, even networked with some advanced computer workstations, making the NMR data processing and analysis much more easy and effective.

For the earlier FT NMR spectrometers, several methods have been implemented to improve their data processing capability effectively. Since current PCs are powerful and popular, one simple and effective updating method is establishing spectrometers' data transferring with the PC through the serial or parallel interface and further data processing on the PC. The hardware has been solved adequately (Zolnai *et al.*, 1990; Humbert *et al.*, 1991; Kasi Viswanathan *et al.*, 1993), the popular data processing software is BRUKER's 1D and 2D WINNMR (Thiele, 1992), but the data processing functions are not sufficient for the wide application purpose.

The package we present here is a PC-based off-line NMR data processing application software system, which presents interactive and easy-to-handle common 1D, 2D NMR, and NMR imaging data processing and an analysis tool for scientific work on current IBM-PC compatible advanced computers. Also a bridge has been set up to link NMR experimental data with other opulent PC application software. Although the package is developed for BRUKER NMR spectrometer, dedicated with ASPECT 3000, it is also suitable with other types of NMR spectrometers with only the simple data format conversion.

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HARDWARE REQUIREMENTS

The WHNMR package runs under MS DOS 3.3, an Intel 80386 microprocessor with 80387 coprocessor, 4 Mbytes main memory, 512 Kbyte video memory, and at least a standard 640*480 VGA adapter. The raw data are transferred from the BRUKER Aspect 3000 computer via serial transfer (such as KERMIT) or parallel transfer (such as ZZNET, FASTRAN).

SOFTWARE SYSTEM

The package includes PCNMRI, PCNMRII, MRIC, and NMRu (four parts), they are the server for 1D FTNMR experimental data (FID) processing, 2D FTNMR FID processing, magnetic resonance imaging (MRI) data processing, and 1D NMR auxiliary application, individually. Since the data format is different in KERMIT and ZZNET transfer, a small accessory program is necessary for conversion.

ASPECT 3000 is dedicated with DISMSL software system to achieve data acquisition, processing, and display. The FASTRAN or ZZNET transferred FID or spectrum files are preferable for their fast transfer rate. Because the BRUKER NMR data are stored in the special 24-bit integer, 48-bit floating point number and 6-bit character formats, all related

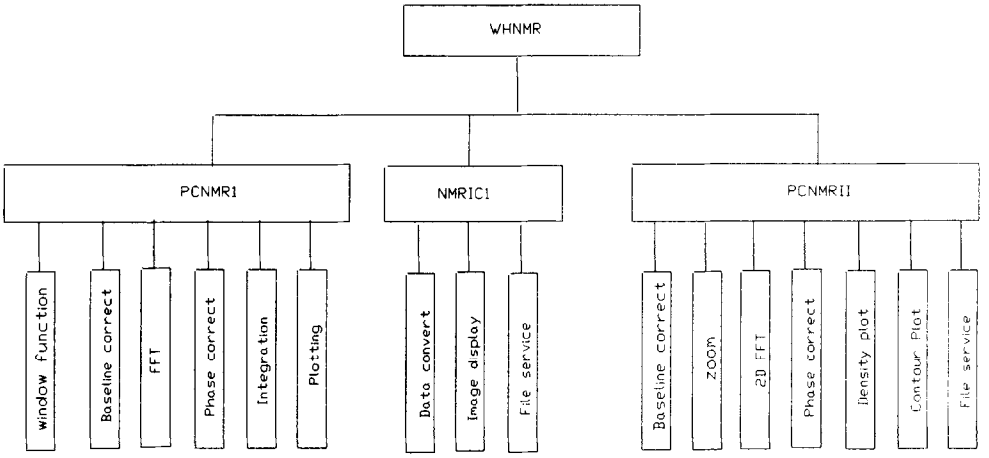

Fig. 1. The structural schematic diagram of WHNMR.

experimental parameters and data are converted automatically when reading the data file.

PCNMRI, coded with TURBOC 2.0, is used for the standard 1D FT NMR data processing. The transferred FID data can be processed with window functions, FFT, peak picking, phase correcting, baseline correcting, calibrate, integration, smoothing, and other functions as a common routine. The user-friendly pull-down menu makes the dialogue interface easy to use. The result can be plotted on HP 7475 plotter.

PCNMRII, coded with NDP ForTran 2.1, is served for 2D FTNMR data processing as a standard routine. The raw 2D data matrix (512*512 points for 4M main memory) can be processed with common

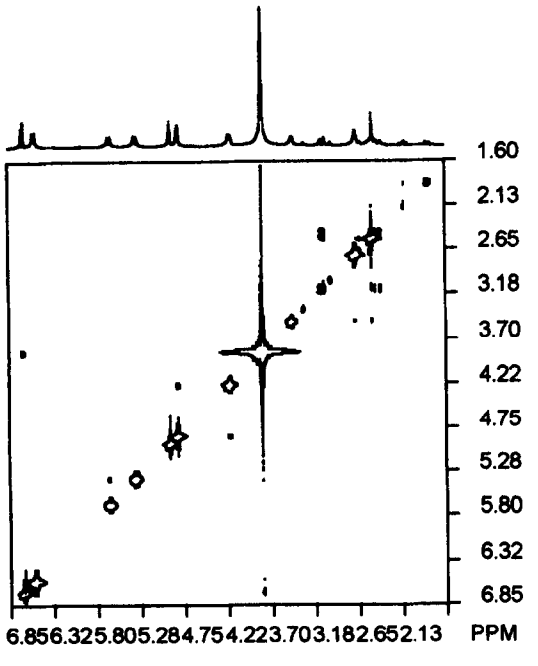

Fig. 2. 400 MHz 2D NOESY spectrum of codeine.

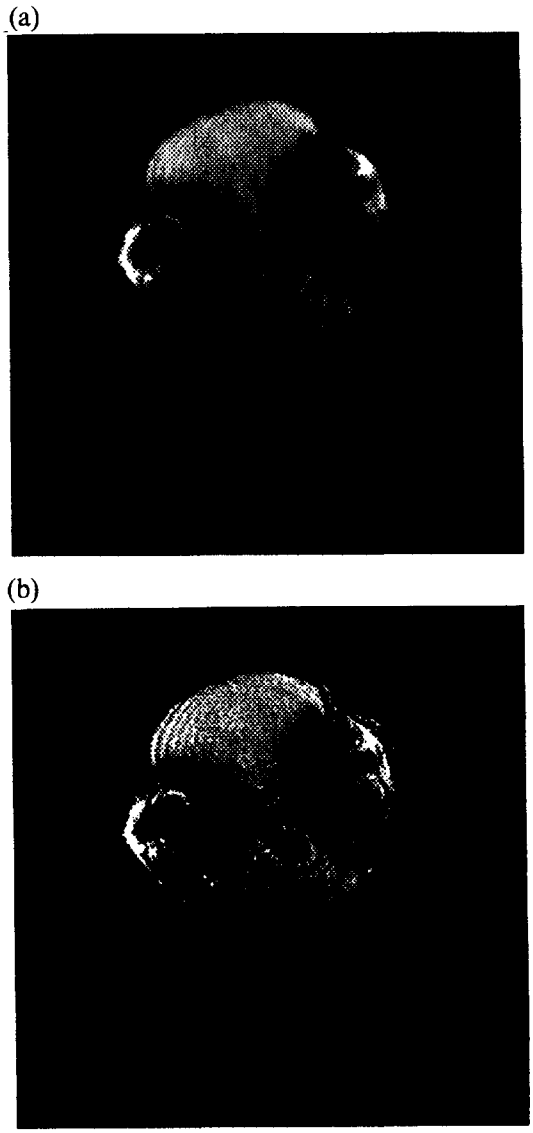

Fig. 3. A slice of mouse brain NMR proton density image: (a) 256-greyscale picture processed with "tonal correct"; (b) 256-greyscale picture processed with "edge enhance".

window functions, FFT in F1 and F2 direction, phase correction, baseline correction, volume integration, etc. Further processing includes density display, zoom, contour display, stacked plot, and projection plot. The processed data can be stored in the compressed or in the PIXI file format (Zolnai *et al.*, 1990). One standard contour plot of a 2D NMR spectrum, taken on a BRUKER MSL400 spectrometer and processed with PCNMRII, is presented in Fig. 2.

MRIC1, coded with TURBO C 2.0, is used for MRI data converting. Since the NMR imaging processing functions of some spectrometers are very simple and limited, and the current advanced PC has excellent image processing application software. It is preferred to convert the MRI image data file to the universal standard image format—the 256-greyscale Zsoft PCX file format, which can be processed with the common image processing functions such as "edge enhance", "trace contour", "tonal correct", "desparcal", and others to assist data analysis via some famous imaging processing system (for example: Aduls PhotoStyler) easily. A slice of a mouse brain NMR proton density image is presented in Fig. 3.

NMRu is used as an auxiliary program for displaying spectrum and converting it to DXF (autoCAD) or HPGL format with the KERMIT or ZZNET transfer protocol.

The PC-based universal NMR data processing and analysis system is available for a wide purpose. Since PC is inexpensive and acceptable in most laboratories and there are a lot of application softwares, this package will assist NMR study and application or act as an educational tool.

Program availability—The executable copies of the programs are available from the author upon request.

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