

Touch NMR: An NMR data processing application for mobile device

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Target audience

The target audience is the NMR researchers who want to process their NMR data with an iPad.

Purpose

As mobile pad is becoming more and more popular, the growing applications on it are bringing us conveniences in daily life. Recently, U.S. Food and Drug Administration has allowed physicians to view medical images on the iPhone and iPad manufactured by Apple Inc.¹. As is known that such medical treatment in CT and MRI can now use software for iPhone/iPad to do the jobs. Based on our homebuilt NMR data processing software for desktop computer, a new version for iPad named Touch NMR was released out². Touch NMR is attempted to help process NMR data at any time and everywhere.

Introduction

Touch NMR can handle data from Agilent, Bruker and JEOL NMR spectrometers, and accomplish the basic functions: FID operations (shown in Fig.1), FFT, manual/automatic phase correction, automatic baseline correction, referencing, integration (shown in Fig. 2), T1/T2 fitting (shown in Fig. 3), DEPT edit (shown in Fig. 4), 2D contour view (shown in Fig. 5), 2D projection (shown in Fig. 6), graphics exporting and printing and so on. The major difference from traditional software is that Touch NMR takes the advantage of multi-touch technology. There is also a built-in file system which helps user to manage the data imported. Another wonderful function is that cloud storage is introduced in. User can choose to use the popular cloud providers such as Dropbox to store the data for exchange and update.

Operations

Touch NMR implemented four orientations' control. User can rotate iPad to the appropriate direction. All operations can be accomplished with multi-touch. In Touch NMR operations with one finger, two fingers or three fingers have different functions. Tapping the spectrum shows or hides the toolbar. Pinching with two fingers zooms the spectrum. Swiping left with three fingers displays the full spectrum and swiping right does the spectrum height adjustment. Such kinds of operations save researchers much time in their daily jobs.

Acknowledgements

Since the first version of Touch NMR published in Oct. 2012, there are more than 1,500 downloads in App Store from worldwide. In the meantime we got many valuable suggestions that help us improve the application. And many more functions will be introduced in the later updates. This work was partially supported by the NNSF of China (No. 81101037) and Nanjing Military key projects in medical technology innovation (No. 09Z019).

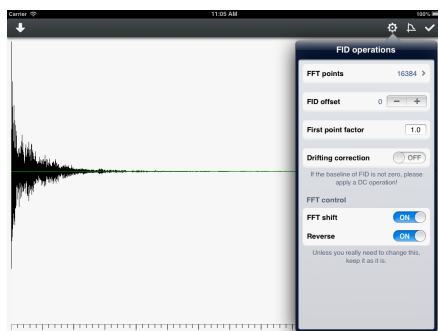


Fig. 1. FID operations: FT points, first point and drifting corrections, and so on.

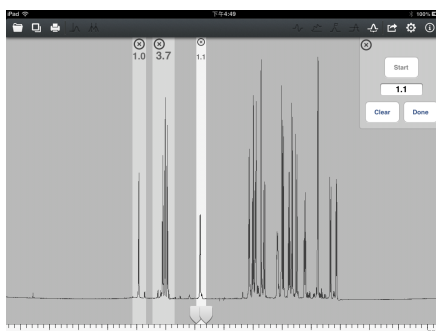


Fig. 2. Swepting to select the region to do the integration.

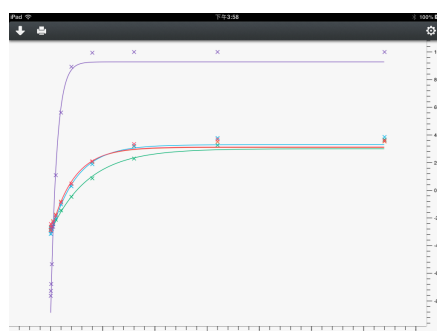


Fig. 3. T1 (or T2) fitting can be generated after user picks out the peaks.

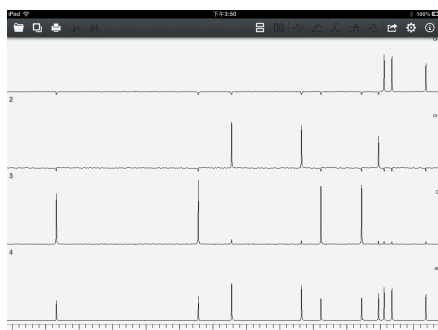


Fig. 4. DEPT edited spectrum from 3 or 4 1D spectra or an arrayed spectrum.

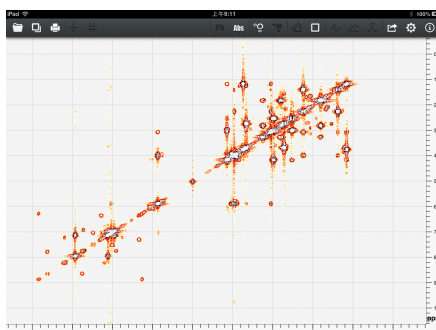


Fig. 5. Contour view of 2D spectrum.

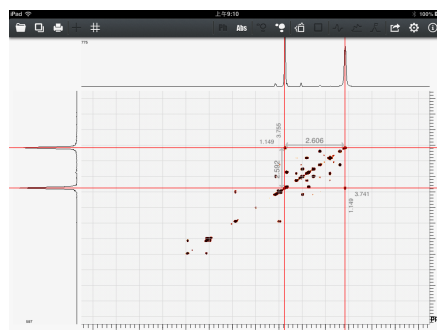


Fig. 6. Projections of 2D spectrum in both F1 and F2 dimensions.

References

1. FDA clears first diagnostic radiology application for mobile devices. <http://www.fda.gov/NewsEvents/Newsroom/PressAnnouncements/ucm242295.htm>, 2012-2-4.
2. Touch NMR, software copyright register number: 2013SR028942.