Automatic Peak Finding of Dynamic Batch Sets of Low SNR In-Vivo Phosphorus NMR Spectra

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INTRODUCTION:

A major problem of in-vivo nuclear magnetic spectroscopy (MRS) is the large amount of data that can be obtained which requires time-consuming post-processing[1]. Many computer automated methods[1-10] have been developed to assist with the various levels of the post-processing of MRS. These algorithms and related software packages suffer from one or more of the following: (a) not user friendly, (b) needed considerable operator intervention, (c) difficult to implement, (d) cumbersome to maintain, (e) relatively slow and (f) inaccurate for spectra with low signal-to-noise-ratio (SNR), overlapping peaks and large dynamic changes.

Toward the final goal of a method so fast and automated that the results would be available almost before the patient left the magnet, we set out developing an algorithm for automated post-processing of P^{31} skeletal muscle spectra. The program at its current state will automatically identify each peak of a P^{31} skeletal muscle spectrum consisting of an external standard (HCCTP: hexachlorocylcotriphosphazene in benzene and chromium acetate), phosphomonoester (PME), inorganic phosphate (Pi), phosphodiester (PDE), phosphocreatine (PCr), γ-, α-, and β-adenosine triphosphate (ATP).

METHOD:

The automated algorithm was set up to deal with the specific type of P^{31} spectral data that we obtain from our in-magnet exercise studies of peripheral vascular (PVD) and cardiac disease patients. The data is typically structured as a set of 32 to 52 spectra each representing 32 seconds (16 averages with repetition time of 2 seconds) acquired during resting, in-magnet exercise, and after-exercise-recovery obtained from the medial gastrocnemius muscle. Each spectrum has eight peaks, as described above. These data sets have fairly low SNR, have dynamic and significant changes in the areas of Pi and PCr, and experience peaks splitting and chemical shift due to pH changes.

Using an average of five resting spectrum for greater SNR, the algorithm first defines the peak positions and a small region around the peak and then runs through the entire data set defining each peak as the highest peak within the small window on the x-axis. The initial peak positions are originally defined by first labeling the PCr peak as the tallest peak in the middle third of the spectrum. Next, the external standard peak is defined as the tallest peak in the region between the farthest left point of the spectrum and half the distance to the PCr peak. The PME, Pi, and PDE peak are defined by their approximate distance from the PCr peak, as determined previously by looking at 20 similar data sets. Finally, using Demetriou's[11] method, a technique new to P^{31} spectra analysis, the three ATP peaks are identified automatically. Demetriou's method[11] decomposes the spectrum into a specific number of increasing and decreasing segments (i.e. each peak is composed of an increasing and a decreasing segment) therefore identifying peak positions without user intervention. The three ATP peaks are found by using 9 segments to map the spectrum from the top of the PCr peak to the right most position. In this way, the first three peaks defined with up and down slopes are assigned as the ATP peaks.

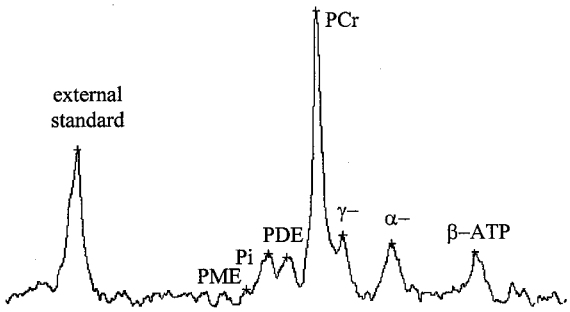

Figure 1: Resting P^{31} Spectrum (spectra 4 out of set of 43) with peak positions defined

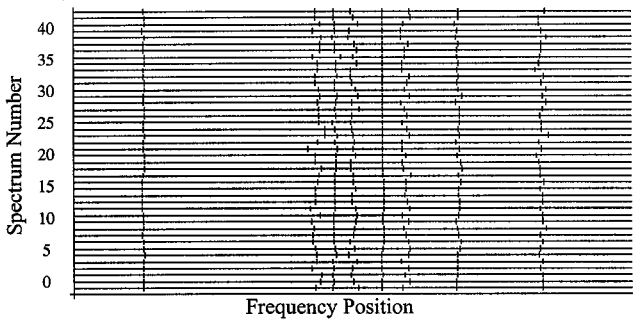

Figure 2: Peak positions determined by the automated algorithm for 43 P^{31} Spectra

The algorithm can run through a set of 50 dynamically changing spectra (including pH changes designated by a Pi chemical shift), in approximately two seconds.

RESULTS:

To test the accuracy of the automated peak picking method, we compared the results of two experts to the output of the algorithm for a total of 1298 spectra consisting of real in-vivo data obtained from in-magnet exercise studies on 20 PVD patients. The experts' experience consisted of two to three years of manual post-processing of large amounts of P^{31} spectra from the same type of in-magnet exercise studies. The computer algorithm was correct at identifying 95% of all eight peaks and 98% of six peaks (if PME and PDE were excluded), when compared to the experts. The two experts agreed with each other 94% of the time when all eight peaks were considered, and 97% when just six peaks were considered (again excluding PME and PDE). Therefore the accuracy of the computer algorithm was as good as the experts.

These results are comparable to Chow's algorithm[7], a method which involves a large amount of expert input amounting to 117 rules. Using similar P^{31} data to test their algorithm (without an external standard), Chow's algorithm was previously found to be 98% accurate when the PME and PDE peaks were excluded[7].

CONCLUSIONS:

The goal of this project is to develop an automated method of spectroscopy post-processing that is both fast and accurate. At this stage, we have developed a program that is accurate at identifying the peak positions, as compared to our two experts.

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