CHEMICAL SPECTRAL ANALYSIS THROUGH SONIFICATION

Joseph W. Newbold

UCL Interaction Center, University College London
London WC1E 6BT
joseph.newbold.14@ucl.ac.uk

Andy Hunt, Jude Brereton

Department of Electronics, University of York
York YO10 5DD
andy.hunt@york.ac.uk,
jude.brereton@york.ac.uk

ABSTRACT

Chemical spectra are an important part of how research chemists analyse the outcomes of experiments. However these complex spectra can be very difficult and time consuming to analyse. This paper outlines an investigation into using sonification to improve the understanding and ease of analysis of chemical spectral data. The project specifically uses sonification techniques to display Nuclear Magnetic Resonance (NMR) spectra. Two sonification methods were designed to offer different perspectives on the data; "Spectral Audification" allows a quick overview of the data while maintaining its subtleties whereas a simple parameter mapping method allows more in-depth analysis of the spectra such as the use of rhythmic patterns to make sets of peaks easily identifiable.

1. INTRODUCTION

Nuclear Magnetic Resonance (NMR) spectra can be difficult to analyse due to both the complexity of the data and the number of spectra which chemists have to analyse. NMR is one of the most used methods for identifying chemical structures. Depending on the organisation and the interaction of the nuclei within a given sample, the NMR spectra can be obtained using a property of possessed by some nuclei known as "spin" [1]. From this produced spectra there are many attributes that a chemist will study to determine what the sample contains, its purity and its molecular structure. This project outlines a preliminary investigation into how sonification could be used to analyse this data and tackle some of the issues with NMR analysis: noisey, complex data with a lot of complexity. By using sound could enable chemists cycle through NMR spectra and find a match faster and easier than with purely visual analysis. The ability to hear sounds in a noisy environment is well know as the cocktail party effect [2] and would be useful for the analysis of spectra and for locating impurities.

1.1. Sonification design for NMR

In order to address some of the issues present in visual analysis of NMR spectra while highlighting important aspects of the spectra, two sonification methods were designed, both offering different perspectives on the data.

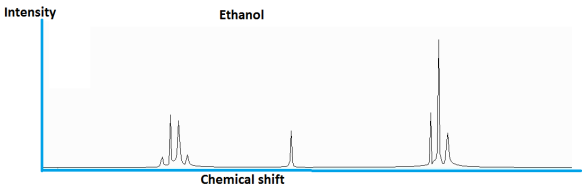

Figure 1: An example NMR spectrum for ethanol. Plotted intensity vs the chemical shift (in parts per million).

As frequency spectra are one of the main contributing factors of an instrument's timbre, by treating NMR in this way each spectrum can be given its own unique sound. It is for this reason this design was termed "Spectral Audification" since, while it is not an audification of the data in the time domain, it can be thought of as frequency domain audification of the spectrum. The set-up used in there preliminary studies, mapped the NMR peaks to frequencies within the audible range to achieve a frequency spectrum for each spectra. By sonifying the data in this way, the entire spectrum can be analysed at once. This makes it very efficient for comparing spectra, as any differences can be heard as a change in timbre.

The second design is a relatively simple parameter mapping to the frequency of a sine wave oscillator. However this simple mapping yields some interesting results due the non-temporal nature of the sonified data. The sonification maps the y co-ordinate to the frequency of a sine wave oscillator, so that more intense peaks have a higher pitch. Additionally due to the nature of the peak splitting caused by the interacting molecular structures in NMR [3], the resultant set of peaks form an identifiable rhythmic pattern. For example, an NMR triplet with each peak equidistant from one another will heard as a rhythmic triplet. This rhythmic information also means that if two similar looking spectra are shifted in chemical shift, their rhythms will not match up if played simultaneously. These designs were chosen to highlight two perspectives of the data, the first giving an overview of this complex data and the second focused more on highlight the specific details of NMR, the collection of peaks, their relation to each other and the effect of the peak splitting [3].

2. TESTING THE SONIFICATION METHODS

From results of an initial pilot test of the potential designs with research chemists, the spectral Audification design was seen as a useful method for quick comparisons. However it was less useful for more detailed analysis involving individual peak detection,

design two however can be used to scroll through the data and locate peaks. In traditional NMR analysis impurities are identified by zooming in on the image, normally substances left over from synthesis e.g. deuterated water. This was the basis for this system's method for impurity location. The data was put through a threshold and anything above the threshold was not played and the points below it were scaled: mimicking the idea of zooming to an image.

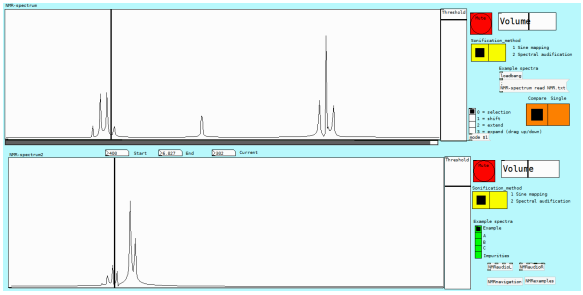

Figure 2: The user interface of the final version of the system with two spectra loaded in, ready for analysis.

To investigate whether using the sonifications for real-life NMR analysis could improve the traditional visual analysis, participants were taken from the University of York Chemistry department The participants were at MChem level or above and with at least one year of experience with NMR analysis. Ten participants aged between 21-25 (mean = 22.8), took part in the test and had between 1-8 years experience with NMR analysis (mean = 5). Participants were given two exercises: a multiple choice identification task and a task to locate two impurities within a given sample. The first task used Ethanol, a relatively simple compound, as its starting point. The participants were then given three options and asked to match the spectra. The two false spectra were altered versions of the Ethanol's NMR and visually appeared similar. The second exercise was designed to explore the impurity detection. Participants were presented with a spectrum that contained two small impurities with the task to locate both impurities. After the completion of both tasks, the participants were given a final questionnaire, the purpose of which was to gain an overall evaluation of the system and project as a whole.

2.1. Results and Discussion

The results demonstrate the use of the sonification system for NMR analysis. The performance of the system for the identification task demonstrates how the designs can be used effectively to distinguish between very similar spectra, with a 60% success rate. In the impurity exercise, all participants were able to successfully locate both impurities, using the impurity detection tool. This aspect was also described as one of the best features of the system by 8 of the participants. From the questionnaire results, an overall positive reaction to the system was seen. All participants agreed to some degree that the system was intuitive and made the given tasks easier, and the majority of users did not find the system mentally straining (80%). the sounds produced were deemed easy to listen to and useful by the majority of participants. Overall, 90% of the participants said they would consider using this system in their NMR analysis in the future.

3. CONCLUSIONS

This project investigated how sonification could be used to ease the analysis of NMR spectra. It would found in these preliminary studies that it could in fact prove a great help to research chemists, who work with these complex spectra on a daily basis. The methods described above aim to provide two differing perspective on the data. One aims to provide an overview of the spectra leading to quick comparisons of spectra and the ability to hear differences in given spectra easily. The second is geared toward a more in depth analysis, allowing for the location of individual peaks and the hearing of split peaks rhythmically. In these initial tests of the methods, their potential for use in NMR analysis it was found that in tasks designed to emulate real analysis tasks, chemist were able to use the given methods to analysis the spectra and found the system intuitive and useful. In future work further studies are needed to asses the system with more complex spectra, as the current studies may have been too simple to properly test the system and to compare the use of the system to the traditional visual analysis.

4. ACKNOWLEDGMENT

This project was completed as part of a Masters project at the University of York's Audio Lab in the Electronics Department. We would like to thank Prof Ian Fairlamb & Joshua Bray at University of York's Department of Chemistry for all their help in this project.

5. REFERENCES

[1] J. Hornak, *The Basics of NMR*. Rochester, NY: J.P. Hornak, 1999, ebook.

[2] E. Cherry, "Some Experiments on the Recognition of Speech, with One and with Two Ears," *The Journal of the Acoustical Society of America*, pp. 975–979, 1953.

[3] R. Hoffman. (2009) What is NMR. [Online]. Available: http://chem.ch.huji.ac.il/nmr/whatisnmr/whatisnmr.html[AccessedNov.11,2013]