Interactive Redesign of 31P-MRS Spectra Visualization Using Jupyter Notebook in Google Colab for Enhanced Neurometabolic Interpretation.

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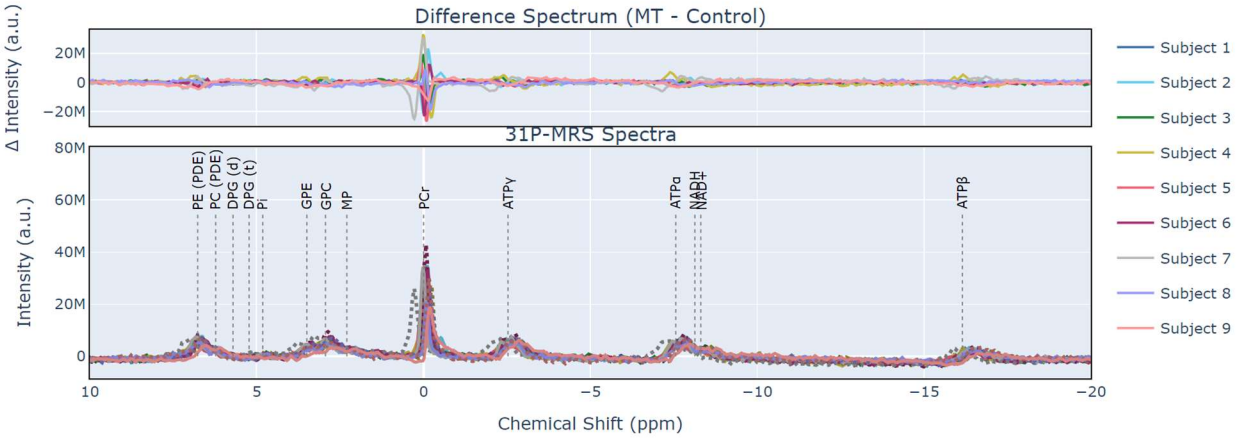

Figure 1: Proposed 31P-MRS Spectra Visualization

Abstract

This paper proposes an interactive redesign of 31P-Magnetic Resonance Spectroscopy (31P-MRS) using Jupiter Notebook in Google Colab for Neurometabolic Interpretation. The redesign incorporates a one-column, two-row interactive Plotly-based graph with four segments: the difference spectrum, 31P–MRS spectra, an interactive Legend, and an interactive bar. Vertically dotted line called Metabolite markers were annotated and used to signal the presence of metabolites at resonating regions. Chemical shift alignment was used for cross-spectra comparison, and enhanced color mapping strategies using Tol's palettes and Okabe-Ito's palettes for perceptually distinct categorization, and color-blind safety. The solution also introduces visual and statistical comparison between conditions (control vs. MT) using grouped bar charts and a paired t-test to ascertain the significance of peak ratio difference. The visualization environment promotes accessibility, reproducibility, and interpretive clarity, enhancing its application for neurometabolic assessment by both educationists and clinicians.

Index Terms: Neurometabolic Analysis, 31P-MRS Spectra

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1 Features of the Proposed Spectra Visualization

The proposed 31P-MRS spectra visualization is divided into four segments: the 31P-MRS spectra, interactive Legend, Difference spectrum, and interactive Menu.

1.1 31P-MRS Spectra Segment (Lower Left)

The Spectra overlay segment (Figure 1), has nine (9) subjects or spectra pairs. For each pair, one represents the Control condition identified by a dotted spectrum curve. The other represents the MT (Magnetization transfer) condition identified by a solid spectrum curve. The use of colored, dotted and solid lines enhances the visual perception of the spectra as belonging to different groups, conforming to the Gestalt principle of similarity[1] and color vision deficiency[2]. Within the spectra segment are vertically dotted lines called metabolite markers (Figure 1), used to identify unique metabolites. These markers exist in resonating regions where distinct signals from metabolites are observed. Abbreviations of metabolites are used to label the top of each Marker (Figures 1) and are called metabolite annotations. Analyzing the signal characteristics such as intensity, shape, and position helps in identifying, quantifying, measuring, and comparing metabolites,[3, 4]. A feature known as details-on-demand or tooltip (Figure 2), is used to access details of peaks and other points along the spectra. The tooltip displays information about signal characteristics of metabolites (intensity, shape, position) for straightforward interpretation.

1.2 The Difference spectrum (Top left)

Second, the plot also features a Difference spectrum segment (Figure 2), which highlights metabolic changes induced by saturation, revealing metabolic activities. For MT – control (Figure 2 below), a relatively wide positive difference is signified by a high peak in the upward direction. A relatively wide negative difference is signified by a high peak in the downward direction. Relatively identical or near identical conditions produce flat or low peaks. The size of the change can be measured by the area under the peak in the difference spectrum.

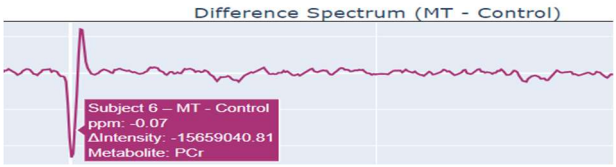

Figure 2: Difference spectrum with sample tooltip.

1.3 Interactive Legend segment (right)

Third, the interactive legend has buttons of distinct colors representing nine (9) subjects. Each legend button controls the automatic toggling (Activation/Deactivation) of spectra display, namely, the control, the MT, and the difference (MT - control) for the subject it represents. Double-clicking on any legend button deactivates all buttons (except the button that was double-clicked) and the corresponding spectra display from the plot, leaving only the spectrum for the item that was double-clicked. Repeating the process reactivates all legend items. This double-clicking effect helps to filter per Subject spectra display for comparison and analysis.

1.4 The Interactive Bar (Top right)

The download as PNG icon allows you to download and save your visualization, the Zoom button allows you to click and hold the mouse button, then drag to highlight, and release the mouse button to execute the zoom effect.

2 Results

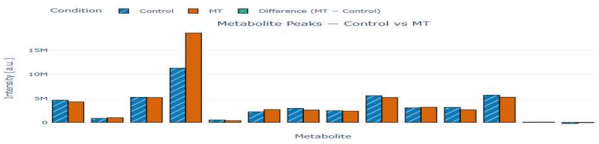

Figure 3: Metabolite peak average comparison.

On one hand, Figure 2 above shows average peak comparison across all subjects for each metabolite, between conditions (mean_MT vs mean_control), while figure 3 below shows the corresponding average difference (mean_MT – mean_control). Using t-test, the difference, the t-statistics and the p-value (see Table 1 of the figures and tables file) shows that at 0.05 level of significance, no metabolite showed any significant difference between control and MT. While PCr has a large difference (7.3 million), the t-statistics is still low due to relatively high variability.

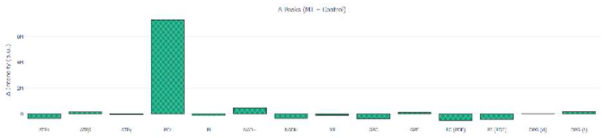

Figure 4: Peak mean Difference (MT - control)

On the other hand, the target is on biologically meaningful derived ratios or composite metric. Figure 5 below shows average metabolic ratio comparison between conditions. For example, Pi/PCr decreased by about 67%. PCr/ATP_total increase by 74% and Pi/ATP_total decreased by 113% (indicating reversal). This is a descriptive summary of metabolic shift.

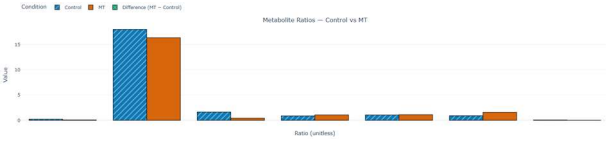

Figure 5: Metabolite ratios average comparison

Figure 6 below shows corresponding difference (mean_MT – mean_Control). Using a paired t-test at 0.05 level of significance, shows all p-values > 0.3. This means changes are not statistically reliable, though biologically interesting with the sample size n=9. Hence the need for larger n. See tables 3 and 4 in figures and tables file.

Figure 6: Ratio difference.

References

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