Spectrascope: An Interactive Redesign of Multi-subject MRS Visualization and Metabolite Ratio Analysis

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ABSTRACT

The current MRS data visualization provided by the Bio+MedVis 2025 Challenge is static and non-interactive, lacks clarity, does not support cross-subject evaluations, complicates the calculation of metabolite ratios, and prevents the analysis of multi-subject spectra. These factors make it difficult for researchers and clinicians to interpret and analyze ^{31}P-MRS brain spectra. Therefore, we propose a SpectraScope which is an interactive, two layered, multi-subject MRS visualization tool that addresses the limitations of current visualizations provided by the Bio+MedVis 2025 Challenge. The proposed visualization displays any number of subject spectra, enabling comparisons between subjects or between a subject at time points. This tool simplifies metabolite ratio calculations, displays all subjects simultaneously, enables users to switch either group-level or single-subject and a time point analysis, highlights and annotating known metabolite peaks, provids interactive zooming and panning for peak inspection, calculats and displays metabolite ratios for a selected subject relative to PCr using a bar chart. All these features improve the understanding and analyzing of ^{31}P-MRS data and metabolite ratio by researchers and clinicians.

Index terms: Biomedical Data Visualization, Spectral Analysis, Metabolite Quantification, Metabolic ratio analysis, MRS data

1 INTRODUCTION

The early detection and diagnosis of neurological disorders is essential to the treatment of Alzheimer's and Parkinson's diseases[4]. Magnetic resonance spectroscopy (MRS) and magnetic resonance imaging (MRI) are two essential techniques for imaging and assessing biochemical processes in living and vital tissues. In particular, Phosphorus-31 Magnetic Resonance spectroscopy(^{31}P-MRS) enables the identification and quantification of high-energy phosphate metabolites such as PCr ATP, and Pi which play a vital role in cellular energy metabolism[2,3]. The conventional visualization of MRS data or spectrum plotting presented by the Bio+MedVis 2025 Challenge is typically single subject, static, lacks labeling for known metabolites, lacks comparative analysis, makes metabolite ratio calculations difficult, and lacks interactive functionality, limiting its use in research and clinical diagnostics[5]. We present a two-layered interactive visualization that helps researchers and clinicians interpret MRS data and make better decisions in metabolite analysis

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2 PROPOSED DESIGN

To support researchers and clinicians in analyzing metabolites, we propose **SpectraScope**—an interactive, layered visualization tool designed to improve understanding and aid decision-making in metabolite analysis. The proposed method for visualizing MRS data has two graphs: ^{31}P MRS Spectrum graph, shown in Figure 1(Top), and the Metabolic Ratio Analysis graph, shown in Figure 1(Bottom). The former displays the chemical shift spectra for each subject at time point's t0 and t1. Whereas the latter represents the metabolite ratio peak areas relative to a reference PCr. Generally, the proposed SpectraScope visualization has the following goals.

- Enabling the visualization of all 9 subjects simultaneously.
- Enabling users to switch either group-level or single-subject and a time point analysis by allowing the user to add, remove, or toggle subjects within a single view.
- Highlighting and annotating known metabolite peaks.
- Providing interactive zooming and panning for peak inspection.
- Displaying metabolite ratios relative to PCr using a bar chart.

2.1. ^{31}P-MRS Spectrum Visualization Graph

The line plots in the ^{31}P MRS Spectrum Visualization graph (see Figure 1(Top) helps researchers and clinical workers to easily navigate, detect, compare and analyze cellular metabolism and oxidative stress. This graph can provide the following interactive features.

- **Zooming**: zooming in and out enlarges or reduces the selected spectral region, helping to resolve clutter and enhance visualization (Figure 2(c) in the supplementary materials). This is essential for analyzing and comparing metabolites within or across subjects.
- **Panning**: When zoomed in, parts of the spectrum may be hidden (Figure 2(e) in the supplementary materials). Panning lets us move around the graph horizontally or vertically without altering the data.
- **Legends**: Each subject in the spectrum is shown as a colored line with a label. If a subject has both t0 and t1, they share the same color: t0 is a solid line and t1 is dashed (see Figure 2(Top) in the supplementary materials). Clicking a legend line toggles that subject's visibility, making it easier to compare spectra within or across subjects.
- **Slider**: Located next the spectrum graph(Figure a(Center), the slider lets users scroll horizontally to view specific regions of the MRS spectrum (see Figure 2(b) in the supplementary materials).
- **Mouse hover**: Hovering over a spectrum line shows detailed information (see Figure 2(d) in the supplementary materials).

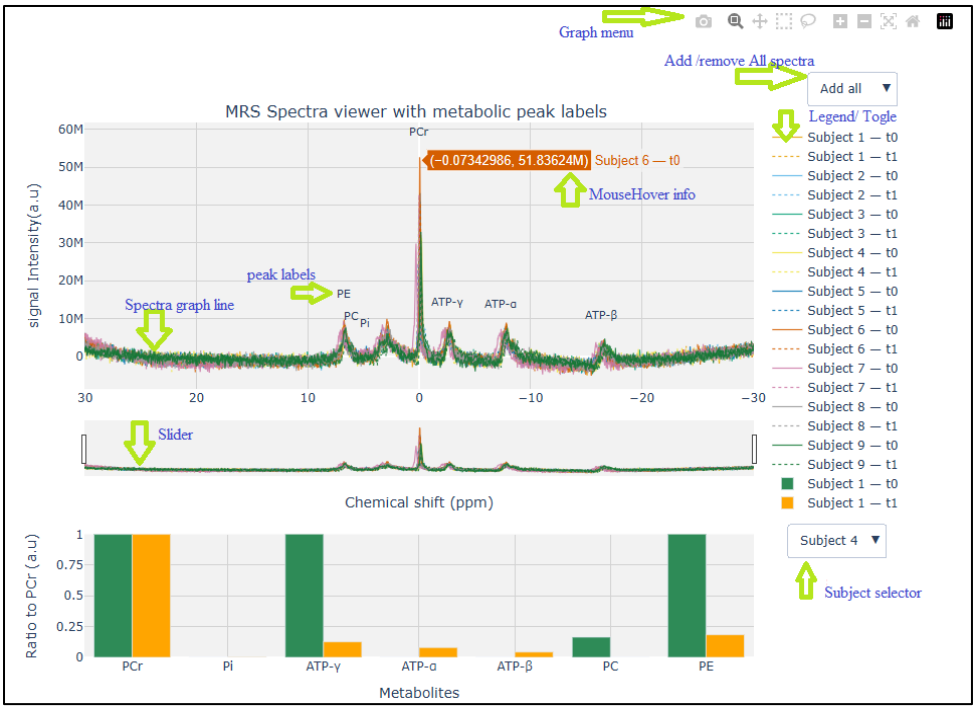

Figure 1: Interactive visualization of MRS data. The spectra viewer (top) displays metabolic peaks with labels, subject selection, and interactive tools for adding/removing spectra. The bar graph (bottom) shows metabolite ratios relative to PCr for the select.

2.2. Metabolic Ratio Analysis

Metabolite ratios are computed using the area under the curve (AUC) within specific chemical shift windows (e.g., PCr: ~0 ppm, Pi: ~5 ppm)[3]. ^{31}P-MRS metabolic ratios are used to assess the relative concentrations of phosphorus-containing metabolites in tissues like brain, liver and muscle[1,2]. Researchers and clinical workers can use the metabolic ratio analysis graph to explore complex spectroscopy data, draw insights, and support evidence-based conclusions. The metabolic ratio analysis graph shows the ratios of all metabolites for the subject you select from the combo box as shown in Figure 1(bottom). The metabolic ratios which displayed in the bar chart, help the researchers and clinicians to identify, compare, and summarize values, as well as assess metabolic health for treatment decisions. Generally, the metabolic ratio has the following advantage:

- Comparison of metabolite peak area ratios relative to PCr across two time points (t0 and t1).
- It enables comparison of metabolic states between subjects or across time points (e.g., before and after an intervention).
- Ratio-based visualization reduces the impact of scanner noise or scaling inconsistencies.
- Deviation from expected ratio can indicate underlying biochemical or neurological disorder.

2.3. Implementation Details

We use a python based framework called Plotly tool, and plotly.express libraries for implementing the proposed visualization graph. In addition to these we also use supporting tools like pandas, numpy and scipy, signal. These allows researchers to load their own datasets.

3 Conclusion

This work addressed the limitation and challenges of MRS data visualization provided by Bio+MedVis 2025 Challenge using two separate graphs: ^{31}P-MRS Spectrum Visualization graph and metabolic ratio analysis graph. Each graph is designed to be used either independently or in combination. The proposed visualization incorporates several analytical and navigation features, including zooming, hovering, panning, tooltips, access on demand, and toggling. Finally, it is worth noting that the dual-layer spectral graph improves the understanding and analysis of metabolic changes or oxidative stress.

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