Interactive Visual Analytics for Magnetic Resonance Spectroscopy Data

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Abstract

Magnetic Resonance Spectroscopy (MRS) is a non-invasive technique for quantifying metabolite concentrations in biological tissue, offering crucial insight into neurological and metabolic conditions. The IEEE BioVis 2025 Redesign Challenge calls for improved visualization tools to support the interpretation of this complex data. We present an interactive web-based platform built with Dash and Plotly for the exploratory analysis of P-MRS data at both individual and cohort levels.

Our tool combines preprocessing (including chemical shift alignment), feature extraction (e.g., SNR, FWHM, symmetry), and linked visualizations such as spectral plots, correlation heatmaps, dimensionality reduction, and metabolite ratio comparisons. Design choices follow principles of progressive disclosure, interpretability, and reproducibility, enabling users to navigate from raw spectra to cohort-level trends while maintaining clarity and usability.

Index Terms: MRS, P-MRS, Spectroscopy

1 Introduction

Neurological conditions are a leading cause of disability and death worldwide, and early detection is critical for improving patient outcomes. Magnetic Resonance Spectroscopy (MRS) is a non-invasive imaging technique [2] used to measure metabolite concentration within biological tissues, offering insights into neurodegenerative diseases, cancer, and other metabolic abnormalities. Unlike traditional Magnetic Resonance Imaging (MRI), MRS trades spatial information for chemical information, analyzing metabolites that can be analyzed by its chemical shift, which is its difference in resonance frequency relative to a particular reference metabolite, in our case, 31P-MRS[3].

31P-MRS is captured in a voxel structure, and basically boils down to the spectral peaks and graph, and interpretation for meaningful relationships are difficult to understand, problems that are largely unmet in current clinical tools, with a focus on 1H-MRS. The goal of this tool is to bridge this gap by providing an interactive, visual analytics platform tailored to 31P-MRS data.

2 Application Overview

The developed application is an interactive web-based platform built with Dash and Plotly to support an extensive exploratory analysis of 31P-MRS data. The application enables users to upload a spectral and a base chemical shifts file, process said data, view and compare metabolite features across individual subjects, and perform advanced statistical and visual analyses. Core functionality includes spectrum alignment (With Chemical Shift correction), metabolite feature extraction, PCA dimensionality reduction, ratio-based comparisons, and 2D and 3D plotting of comparisons and correlations between features. The interface is designed for clarity, modularity, and progressive exploration.

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3 Visualization Techniques

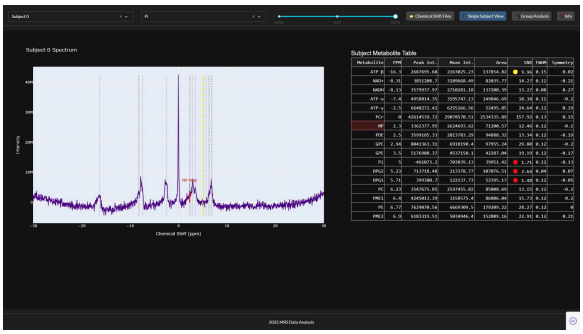

Figure 1: UI layout and single subject analysis

The application provides a suite of visualizations designed to support both detailed single-subject inspection and group-level pattern recognition in P-MRS data. These tools expose all relevant metabolite features and enable intuitive, domain-specific exploration. Each visualization supports key statistics, including peak intensity, mean, standard deviation, area under the curve (AUC), and signal-to-noise ratio[1] (SNR) as shown in Figure 1, making feature-level understanding and comparison accessible and interactive.

Different Metrics reasoning

Full Width At Half Maximum (FWHM) measures the line broadening and how the peak is formed. Narrower peaks typically indicate better spectral quality, it is a qualitative measure. Signal To Noise Ratio (SNR) Determines how well can a signal be interpreted;[1], SNR values below 3 to 5 are agreed to be too low for significant measurements [4], and depending on the sample, bigger values are needed. Symmetry analyses how well formed a peak is, and is also a quality measure of the signal.

Selection tools

Users can dynamically filter data by metabolite, subject, or chemical shift tolerance (ppm), with a tunable range from 0.025 to 0.075. These filters enable targeted analysis across all visualization modes.

Spectral Visualization and Alignment

Spectral plots are available for both single-subject and cohort-wide views. PCr-based chemical shift correction is applied to resolve positional inconsistencies in peak locations. Testing revealed peak misalignment in some subjects (e.g., 6 and 12) where PCr peaks did not align with the 0 ppm reference. Visual inspection of the provided CSV confirmed that correction was not pre-applied, motivating the inclusion of a PCr-based alignment step. This standard yet critical correction step ensures accurate downstream analysis.

Feature Table and Metrics

An interactive metabolite feature table presents both subject-specific and group-average metrics. Extracted features include peak

intensity, mean intensity, AUC (Area under Curve), FWHM (full width at half maximum), SNR (Signal To Noise Ratio), and a custom symmetry metric. The table updates in real time with user selections and PPM window adjustments.

Group Distributions and Outlier Analysis

Boxplots, violin plots, and bar graphs illustrate the distribution of metabolite features across subjects. Hover interactions reveal subject-level details, allowing users to identify trends, deviations, and outliers within the group.

Clustering and Dimensionality Reduction

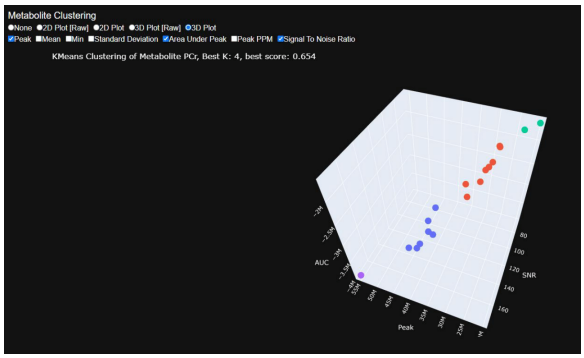

Figure 2: 3D clustering with User-selected information

To uncover latent patterns in the data, the application includes both 2D and 3D projections using Principal Component Analysis (PCA). These can be based on raw spectra or selected features above the desired dimensionality of the plot. KMeans clustering with silhouette-based optimal overlays is used to identify separable subgroups as shown in figure 2, with all plots being interactive, with subject IDs and cluster membership available on hover.

Metabolite Comparison and Ratio Analysis

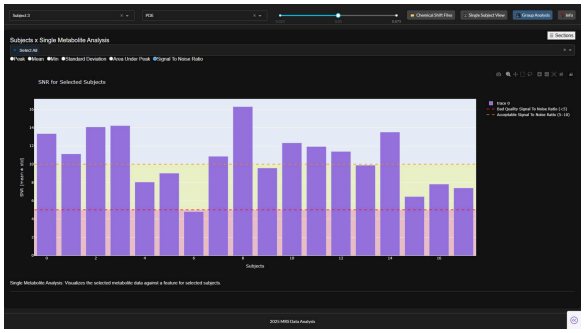

Figure 3: Subjects x Single Metabolite Analysis: SNR

Users can compare the behavior of a selected metabolite across all or chosen subjects such as shown in figure 3. Additionally, the metabolite ratio module (e.g., Pi/PCr) visualizes bar, box, and violin plots for ratio-based comparisons, enabling insight into metabolic balance across individuals.

Correlation Analysis

A correlation heatmap visualizes inter-subject relationships based on metabolite features, helping reveal similar metabolic profiles and subject clusters.

4 Design Justification and Visualization Theory

The interface was designed with progressive disclosure principles to minimize the cognitive load by separating tasks into scrollable and toggleable sections. A consistent visual grammar—such as fixed axis scales, consistent color mappings, and deliberate spatial separation—enhances interpretability. The dropdown-driven UI reduces visual clutter while preserving user agency and control.

Linked views are deliberately limited to core controls (subject, metabolite, and PPM selection) and table-to-plot interactions. This decision was guided by usability and performance concerns, balancing interactivity with interface simplicity and responsiveness.

5 Performance

The application performs well with the real-world dataset provided for the BioVis Redesign Challenge. Although preprocessing and feature extraction are heavy tasks (especially for larger files), interactive features such as spectrum visualization and table updates remain responsive. For the scope of the challenge and the volume of data used, overall performance is acceptable and does not hinder the workflow.

6 Conclusion and Future Work

Our tool enables in-depth exploration of MRS data through interactive, useful, and grounded visualizations. The main core redesign goals were addressed by integrating preprocessing, feature extraction, and intuitive visualization techniques within a clean and responsive interface. While CSV export and more advanced features could be added in future works, the current implementation successfully meets the challenge scope and the 31P-MRS investigation goals.

7 Acknowledgments

In accordance with IEEE guidelines, portions of this manuscript were revised with the assistance of OpenAI's ChatGPT and Grammarly to enhance text readability, grammar and coherence. The author bears full responsibility for the content and accuracy of the manuscript as well as the design of the tools, software and images.

References

[1] A. D. Hendriks, W. J. van der Kemp, P. R. Luijten, N. Petridou, and D. W. Klomp. Snr optimized 31p functional mrs to detect mitochondrial and extracellular ph change during visual stimulation. *NMR in Biomedicine*, 32(11):e4137, 2019. e4137 NBM-18-0171.R2. doi: 10.1002/nbm.4137 1

[2] A. Santos Diaz and M. Noseworthy. Phosphorus magnetic resonance spectroscopy and imaging (31p-mrs/mrsi) as a window to brain and muscle metabolism: A review of the methods. *Biomedical Signal Processing and Control*, 60:101967, 07 2020. doi: 10.1016/j.bspc.2020.101967 1

[3] F. J. A. Stephan Ulmer, Martin Backens. Basic principles and clinical applications of magnetic resonance spectroscopy in neuroradiology. *Journal of Computer Assisted Tomography*, 2016. doi: 10.1097/RCT.0000000000000322 1

[4] M. Wilson, O. Andronesi, P. B. Barker, R. Bartha, A. Bizzi, P. J. Bolan, K. M. Brindle, I.-Y. Choi, C. Cudalbu, U. Dydak, U. E. Emir, R. G. Gonzalez, S. Gruber, R. Gruetter, R. K. Gupta, A. Heerschap, A. Henning, H. P. Hetherington, P. S. Huppi, R. E. Hurd, K. Kantarci, R. A. Kauppinen, D. W. J. Klomp, R. Kreis, M. J. Kruiskamp, M. O. Leach, A. P. Lin, P. R. Luijten, M. Marjańska, A. A. Maudsley, D. J. Meyerhoff, C. E. Mountford, P. G. Mullins, J. B. Murdoch, S. J. Nelson, R. Noeske, G. Öz, J. W. Pan, A. C. Peet, H. Poptani, S. Posse, E.-M. Ratai, N. Salibi, T. W. J. Scheenen, I. C. P. Smith, B. J. Soher, I. Tkáč, D. B. Vigneron, and F. A. Howe. Methodological consensus on clinical proton mrs of the brain: Review and recommendations. *Magnetic Resonance in Medicine*, 82(2):527–550, 2019. doi: 10.1002/mrm.27742 1