Deep Learning Based GABA Edited-MRS Signal Reconstruction

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Abstract. Magnetic Resonance Spectroscopy (MRS) is a non-invasive imaging technique based on nuclear magnetic resonance (NMR) principles. It analyzes the biochemical composition and metabolic processes of body tissues. Edited MRS Reconstruction converts raw MRS data into meaningful spectrum signals, providing valuable insights into cellular metabolism, organ function, and energy production. This process can help understand normal physiology, diagnose diseases, and monitor their progression. Additionally, it enables the extraction of metabolite concentrations, even when hidden by other biochemical compounds with higher concentrations (e.g., gamma-aminobutyric acid, glutamate, and glutamine). This study proposes a dual encoder head self-attention-based deep learning model to reconstruct the Edited MRS signal for acquiring GABA concentration and benchmark the model's performance on simulated raw MRS data from real GABA-edited ground truths. Our model achieves a 95% decrease in Mean Squared Error (MSE), a 70% decrease in Linewidth, a 450% increase in Signal to Noise Ratio (SNR), and a 42% increase in Peak Shape Score compared to the current existing method on the test set. We also illustrate our qualitative results, demonstrating our method's robust and accurate predictions compared to the ground truth. Our approach can help deliver rapid diagnosis and monitoring of neurological disorders, metabolic diseases, and certain types of cancers by providing refined and accurate data on metabolite concentrations.

Keywords: Magnetic Resonance Spectroscopy · Edited-MRS Reconstruction · Deep Learning · Machine Learning · Signal Processing

1 Introduction

Gamma-aminobutyric acid (GABA) is the principal inhibitory neurotransmitter in the human brain. GABAergic inhibition shapes and regulates patterns

of neuronal activity, serving a key role in cortical information processing and plasticity [18]. GABA is present in the brain at millimolar (mM) concentrations and is, in principle, detectable by magnetic resonance spectroscopy (MRS). However, low-concentration metabolites, such as GABA, Glutathione (GSH), etc., are often overlapped by larger signals and cannot be reliably quantified; therefore, researchers and clinicians use spectral editing techniques to simplify the spectrum, selectively revealing signals from metabolites of interest and removing overlying signals of more concentrated metabolites [19]. MEscher-GArwood Point RESolved Spectroscopy (MEGA-PRESS) utilizes a sequence of radiofrequency (RF) pulses and gradients to selectively excite and manipulate specific resonances in the brain by employing a pair of editing pulses, often called "ON" and "OFF" pulses. These editing pulses are designed to selectively modulate the resonance of the target metabolite, such as GABA, glutamate, etc. Then, by taking the difference between the spectra obtained with the ON and OFF editing pulses, the MEGA-PRESS technique effectively isolates the resonance of the target metabolite from other overlapping signals [13]. This is also known as J-difference editing [11]. Another recent work, Hadamard Encoding and Reconstruction of MEGA-Edited Spectroscopy (HERMES) [4], uses a similar ON and OFF signal acquisition strategy to modulate the resonances of the target metabolites of interest. The acquired data is then processed using Hadamard reconstruction algorithms to separate and quantify the signals corresponding to each metabolite. These algorithms exploit the known encoding patterns and the acquired measurements to reconstruct the individual metabolite spectra. The above approaches, despite tackling important aspects of MRS editing, fall short in their reconstruction methodologies and deliver low signal-to-noise ratios (SNR). This can be attributed to MRS signals being weak and prone to noise, limiting the quality and accuracy of reconstructed spectra [14]. Low SNR can lead to reduced spectral resolution, difficulty in distinguishing overlapping peaks, and challenges in accurately quantifying metabolite concentrations [9]. As another shortcoming, current techniques fail to handle various artifacts that can affect MRS data, such as baseline distortions, chemical shift artifacts, and eddy current artifacts [6]. These artifacts can distort the spectral peaks, introduce false signals, and hinder accurate reconstruction. As such, mitigating and removing such artifacts and increasing the signal-to-noise ratio in MRS signal reconstruction remains a challenge. According to our literature review and based on our knowledge, no peer-reviewed work has been published where deep learning has been employed to tackle these specific challenges and developed a model capable of more efficient and accurate edited MRS reconstruction making our study the first of its kind. Hence, our contributions in this study are as follows:

- Aggregate and reconstruct raw MRS data from ground truth GABA-edited MRS scans.
- Create a Dualhead Self-Attention deep neural network to achieve state-of-the-art Edited-MRS signal reconstruction performance.
- Compare and evaluate our generated spectra with existing methods with custom and relevant evaluation metrics.

2 Methods

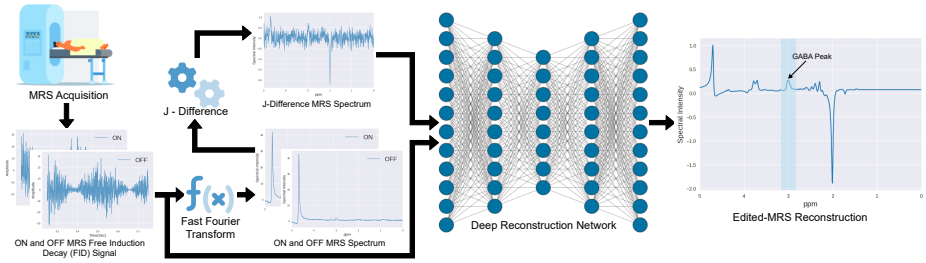

Fig. 1: Overall pipeline visualizing the entire process where it begins with clinicians acquiring MRS data. Subsequently, the ON and OFF Free Induction Decays (FIDs) are transformed into the frequency domain using Fast Fourier Transform. From there, the J-difference spectrum is computed based on the ON and OFF spectra. This J-difference spectrum, along with the ON and OFF FIDs, is then fed into our deep neural network. As a result, the Edited-MRS Reconstructed Signal is generated.

2.1 Dataset

The dataset used in this study has been sourced from the Harris Imaging Lab, University of Calgary [1], with 5000 simulated ground truth GABA-edited MRS signals with their raw MRS Free Induction Decay (FID) signals. For the dataset, the input raw MRS FID transients are generated using a transient maker that adds randomized noises to the ground truth signal that one can expect MRS scans to inherently have while acquisition such as random gaussian amplitude noise, random frequency noise and random phase noise. Then we repeat this process n times and stack them to have n number of different transients. Here, n has been fixed to 40, which is a standard number for real-world scenarios and also keeps our disk size resources in consideration. Now, we have 40 transient FIDs and one ground truth GABA-edited spectra each for 5000 data points. This final dataset is then divided into training and test sets randomly with a ratio of 80:20.

2.2 J-Difference Spectrum

J-difference editing is a magnetic resonance spectroscopy (MRS) technique that enables the selective detection and quantification of metabolites with coupled spin systems, such as J-coupled multiples. It offers a valuable means of investigating specific biochemical pathways or monitoring metabolite levels with diagnostic relevance [11]. In J-Difference editing, two distinct MRS experiments

are performed with different editing pulses applied, in most cases called ON and OFF pulses for each transient. These editing pulses are designed to selectively invert or excite the specific coupled spin system of interest, taking advantage of the J-coupling interactions between the spins of the target metabolite and its neighboring nuclei [21]. The process of getting the spectrum at its core is very simple. First, the MRS FID signal acquisition is performed with the two ON and OFF pulses for each transient, and then the FIDs are converted into the frequency domain using Fast Fourier Transform (FFT) algorithm [16] for both pulses. Then the difference of these signals is taken to get the resulting J-Difference spectrum given by:

$$J\text{–}Difference\ Spectrum = FFT(FID_{OFF}) - FFT(FID_{ON}) \tag{1}$$

In the standard Edited-MRS reconstruction procedures, an average of the J-difference spectrum of all the transients is taken to get the final Edited-MRS reconstructed signal[21, 11]. However, in our case, we take our supervised deep neural network-based approach, explained in the next subsection, and the whole process is also visualized in Fig.1.

2.3 Dual Branch Self-Attention Neural Network

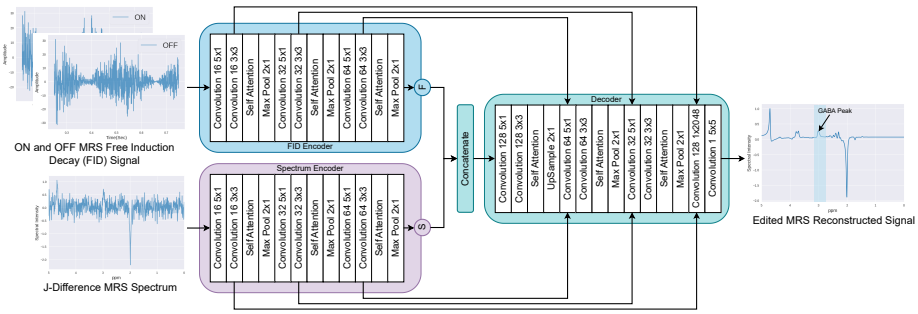

Fig. 2: Detailed architecture of our Dual Branch Self-Attention Neural Network.

To predict/reconstruct the target GABA-edited MRS spectra, we designed a dual-branch self-attention neural network based on an encoder-decoder architecture [3] with skip connections [7] between parallel spatial layers in the encoders and the decoder [20]. The architecture uses two encoders. The first one takes the MRS FIDs with ON and OFF pulses stacked channel-wise, which are in the time domain. The second one takes the J-Difference spectrum in the frequency domain. Both encoders are stacked with Convolutional [17] and max pool layers [15] that convolve and extract features between the transients and on the time/frequency axis, respectively. Also, we introduced Self-attention layers [24]

after each convolutional block in the encoders, which are known to be helpful in extracting dependency information from sequential data. The self-attention is also known as scaled dot product attention and can be given by:

$$Attention = \frac{Softmax(QK^T)}{\sqrt{d_k}} \tag{2}$$

where Q and K are the query and key vectors, d_k is the dimensionality of the vectors, and $\sqrt{d_k}$ is the scaling factor and helps prevent extremely large dot products. Then, the final output of the attention layer is given by:

$$Output = Attention.V \tag{3}$$

where V is the value vector. In self-attention, Q, K, and V are all the same, which is the input to the attention layer. Self-attention mechanisms have proven to be highly effective in neural networks for signal-processing tasks [26, 25, 23, 28]. Unlike traditional convolutional or recurrent layers that rely on fixed local receptive fields, self-attention mechanisms enable capturing global dependencies and relationships within the input data. Self-attention allows the network to focus on the most relevant parts of the signal while considering the interactions between different elements [8]. By assigning weights to different elements based on their relevance and similarity, self-attention mechanisms emphasize the informative components and suppress irrelevant or noisy ones [24].

Our designed architecture also features skip connections, also known as residual connections, which play a crucial role in enhancing the performance and training of neural networks. These connections facilitate the flow of information by bypassing certain layers or blocks of the network and directly connecting them to subsequent layers. Further, deep neural networks often suffer from the vanishing gradient problem, where gradients diminish as they propagate through numerous layers, making it challenging to train deep networks effectively. Skip connections help alleviate this issue by allowing gradients to bypass several layers, providing a direct path for error signals during backpropagation. This facilitates better gradient flow, enabling easier training of deeper networks. They allow information from earlier layers to be preserved and carried forward to subsequent layers and also enable better feature reuse, as the downstream layers can access both the low-level and high-level features captured by earlier layers [7]. By leveraging skip connections, networks can more effectively capture and utilize a wide range of features, leading to improved representation learning and richer feature representations. By providing shortcut connections, the network can more quickly propagate important information across layers, reducing the number of iterations needed for the network to converge to an optimal solution. This can be particularly beneficial when dealing with complex or large-scale datasets [22].

Both the FID Encoder and the J-Difference Spectrum Encoder possess a similar architecture with 3 Convolutional-Self Attention Blocks. Each block has two convolutional layers, one self-attention layer, and one max pool player. The encodings from both encoders are concatenated on the channel axis and fed

into the decoder, which contains 4 convolutional blocks. 3 of the blocks contain two convolutional layers, one self-attention layer, and one upsampling layer. The last output convolutional block only contains two convolutional layers, which generate the final Edited-MRS Signal in the frequency domain. Further details of the architecture design have been visualized in Figure.2. The model was trained for 20 epochs, using the Adam optimizing algorithm with a decaying learning rate scheduler that reduced the learning rate by half after every 2 epochs starting from 0.001, and the batch size was 4 due to memory constraints. However, gradient accumulation was used with a step size of 4, making the effective batch size 16. The loss function used was a mean average error(MAE) [27] with custom loss weights, which forced the model to focus more on the central region where GABA peaks exist (2.8 ppm to 3.2 ppm).

2.4 Evaluation Metrics

In GABA-edited MRS reconstruction, we need to quantify some specific entities. For example, we want our model to look more closely at the section of the subspectra where GABA peaks are supposed to exist. Hence we evaluate the performance of the models on standard and custom metrics, which are as follows:

Mean Squared Error (MSE) MSE is a widely used metric in signal processing to assess the accuracy of a predictive model or an estimation algorithm when dealing with signal data. In signal processing, signals can represent various data types, such as audio, image, time series, or sensor data. MSE provides a quantitative measure of the discrepancy between the predicted or estimated signal and the true signal, making it a fundamental tool for evaluating the performance of signal processing algorithms [2]. Mathematically, the Mean Squared Error is calculated as follows:

$$\frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{x_i})^2 \tag{4}$$

where N is the number of signals in the data, x_i represents the true value of the signal at sample i, and $\hat{x_i}$ denotes the estimated or predicted value of the signal at sample i.

Signal To Noise Ratio (SNR) SNR is a key concept in signal processing that measures the quality and reliability of a signal in the presence of noise. In signal processing, noise refers to unwanted and random fluctuations that can corrupt or interfere with the desired signal. The SNR quantifies the relative strength of the signal compared to the background noise, providing a valuable metric for assessing signal quality [10]. Mathematically, the Signal-to-Noise Ratio is defined as:

$$SNR = \frac{SignalPower}{NoisePower} \tag{5}$$

In this work, we only calculate SNR for the region of interest, that is, the GABA peak that exists between 2.8 ppm and 3.2 ppm in the subspectra.

Linewidth The linewidth, also known as the Full Width at Half Maximum (FWHM), is an important parameter used to characterize the spectral width or frequency resolution of a signal in signal processing and spectroscopy. It represents the range of frequencies or wavelengths over which the signal's intensity is above half of its maximum value. The linewidth provides valuable information about the bandwidth and sharpness of spectral features in a signal. Again, we only calculate FWHM for the region of interest, that is, the GABA peak that exists between 2.8 ppm and 3.2 ppm in the subspectra. This will assess the model's alignment of the subspectra and the reliability of the final quantification [12].

Peak Shape Score We also a peak shape score to measure GABA peak shape similarity using Pearson correlation [5] between the predicted and original spectra to assess subtraction artifacts resulting from improper alignment of subspectra. The shape score is given by:

$$ShapeScore = 1 - PeakSimilarity \tag{6}$$

The final objective is to ***minimize the MSE and the Linewidth*** *and* ***maximize SNR and Peak Shape Score****.*

3 Results and Discussion

This paper demonstrates how deep neural networks can enhance edited MRS signal reconstruction. We also illustrate how adding skip connections and self-attention mechanisms can enhance a deep neural network's capability to extract spatial and sequential interdependence features to perform much well in the end task. We also show how adding a parallel FID encoder branch improves our model's performance to perform the signal reconstruction. Table.1 displays the results of our ablation study on adding these architectural improvements to the base model, and from the performance metrics, we can conclude that our final model that incorporated the spectrum encoder, the FID encoder, skip connections, and the self-attention mechanism performs the best out of all the approaches and significantly much higher compared to the current method of choice, which is the simple average of the J-Difference spectrum. As there were no previous studies or other methods in this domain, we only compared the performance of our model on the Simple Average of the J-Difference spectrum method and the variants of our model using the metric described in Sec.2.4. On the testing set, we observed that the simple average method achieved an MSE of 0.0435, SNR of 0.14, Linewidth of 0.277, and a peak shape score of 0.69. These metrics were comparable to other methods; however still subpar.

Our first iteration of a deep learning model that consisted of only the spectrum encoder and a decoder performed worse in terms of MSE and SNR than the simple average method achieving 0.0735 and 0.02, respectively. However, it achieved better statistics in Linewidth and peak shape score, receiving 0.204 and 0.74. We observe that the model took a significant hit in terms of SNR. On the next iteration of our deep learning model, we added skip connections, essentially improving the transfer of spatial features deep within the network, and hence we achieved much better performance with an MSE of 0.0581, SNR of 0.20, Linewidth of 0.148, and peak shape score of 0.81. We especially improved on SNR from the previous interaction, as expected. Next, We additionally added a self-attention mechanism in the next iteration, and it further improved the performance in all metrics achieving an MSE of 0.0030, SNR of 0.23, Linewidth of 0.082, and peak shape score of 0.95. We observed the jump in performance was higher in MSE, Linewidth, and Peak shape scores. In the next iteration of our model, we introduced a second parallel encoder that encodes the FID signals of the transients, and for ablation purposes, we did not add self-attention in this version. This improved our model's performance by over 100% in terms of SNR by achieving 0.71 on the scale. The MSE was 0.0023, Linewidth was 0.082, and Peak shape score was 0.96. Our final model, which performed the best out of all versions, included the spectrum encoder, the FID encoder, skip connections, and the self-attention mechanisms. This model further improved our SNR by $\sim 9\%$, achieving a ratio of 0.77 and having the least MSE of 0.0020, Linewidth of 0.081, and a Peak shape score of 0.98. Fig.4 visualizes our qualitative results for multiple test data points depicting the ground truth spectrum, the spectrum generated by the currently available method of simple average of J-Difference spectrum, and the spectrum generated by our final model. It clearly shows how close our generated output comes to the ground truth.

4 Conclusion

Edited-MRS reconstruction enables improved detection and quantification of specific metabolites in the brain or other tissues. By selectively manipulating certain metabolite signals, unwanted signals can be suppressed, allowing for clearer identification and measurement of the metabolites of interest. This capability is particularly valuable in studying neurochemical processes and investigating biomarkers related to various diseases and conditions. In this paper, we introduced a Dual branch Self-Attention deep neural network to achieve the task of Edited-MRS reconstruction and achieved state-of-the-art performance as compared to the previous method being used by clinicians, which included taking the simple average of the J-Difference spectrum. The utilization of Edited-MRS reconstruction techniques opens new avenues for advancing diagnostic and therapeutic approaches in various fields. By providing improved sensitivity and specificity in detecting and quantifying specific metabolites, Edited-MRS reconstruction holds promise for more accurate disease diagnosis, monitoring treatment response, and developing personalized treatment strategies. Our only limitation

Table 1: Performance comparison between various models on the test set.

Model/Approach	**MSE ↓**	**SNR ↑**	**Linewidth ↓**	**Peak Shape Score ↑**
Simple Average	0.0435	0.14	0.277	0.69
Spectrum Encoder Only (Base Model)	0.0735	0.02	0.204	0.74
Spectrum Encoder + Skip Connections	0.0581	0.20	0.148	0.81
Spectrum Encoder + Skip Connections + Self-Attention	0.0030	0.23	0.082	0.95
Spectrum Encoder + FID Encoder + Skip Connections	0.0023	0.71	0.082	0.96
Spectrum Encoder + FID Encoder + Skip Connections + Self-Attention (Final Model)	**0.0020**	**0.77**	**0.081**	**0.98**

in this work was the unavailability of extensive in-vivo data. For future work, we want to work with clinicians to create a large benchmark dataset for the same task with high-quality in-vivo Edited-MRS data which we can further work on to tackle challenges with the reconstruction task that we might have missing or not encountered while working with simulated data, such as differences in acquisition techniques due to human errors, or differences due to distinct acquisition equipment.

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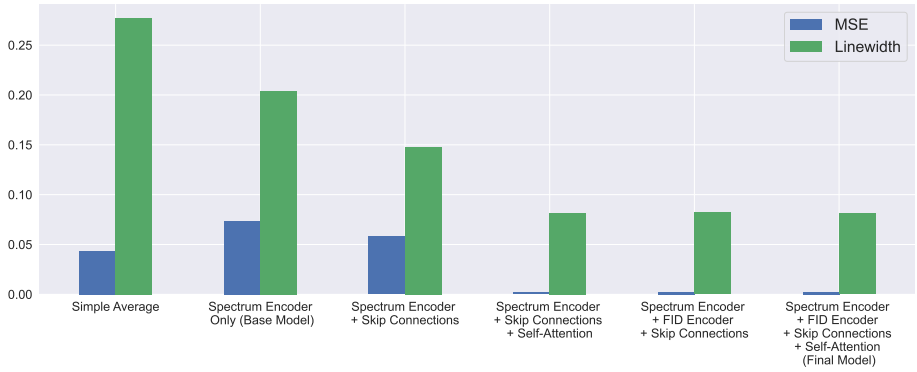
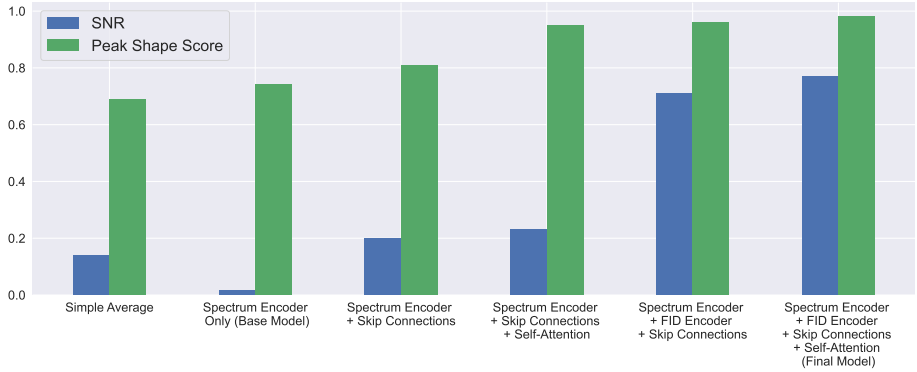


(a) Metrics Minimized



(b) Metrics Maximized

Fig. 3: Bar plots visualizing performance comparison between different models on different metrics.

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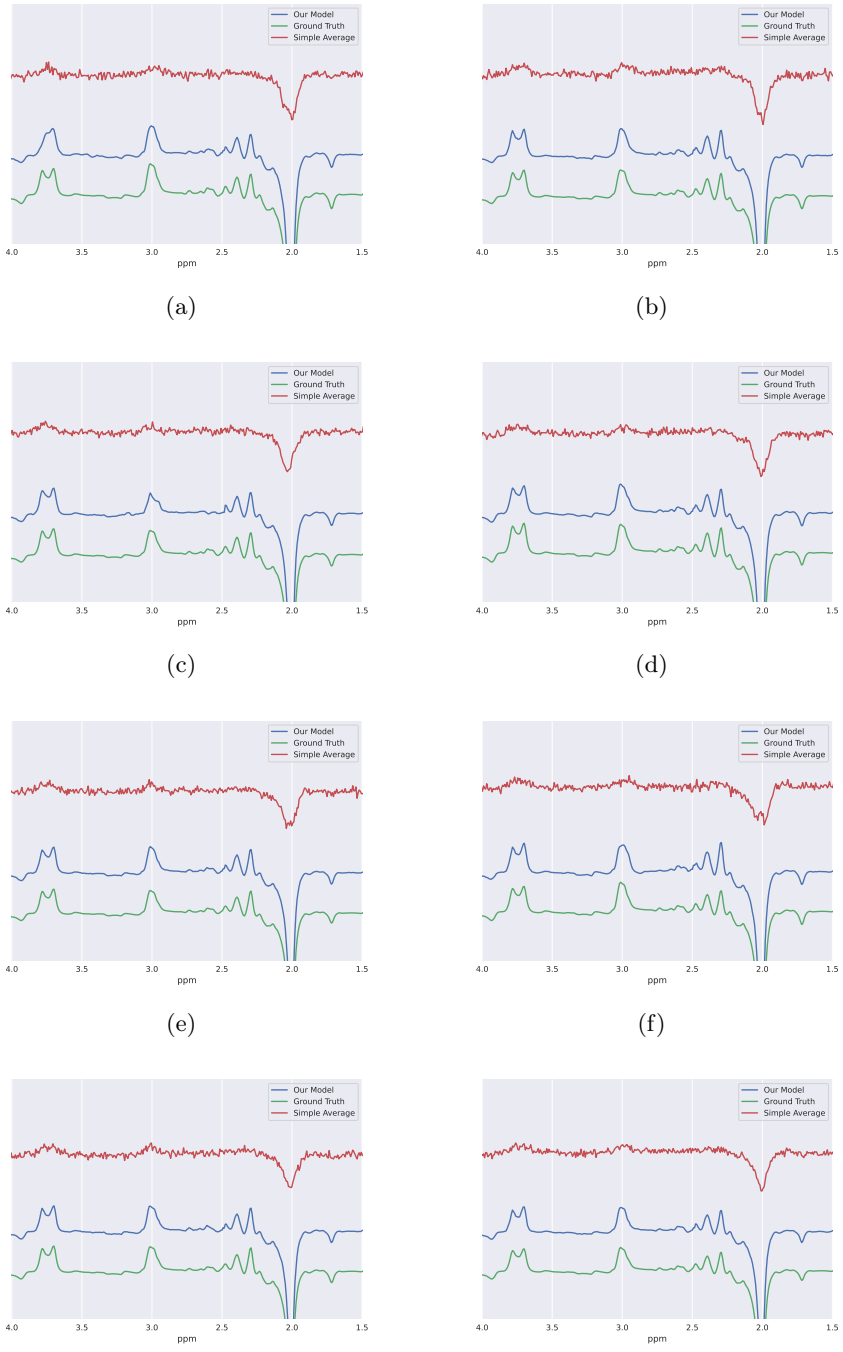

Fig. 4: This figure visualizes the qualitative output of the model on a few test samples comparing the ground truth signal (green), the signal generated from the simple average of the J-Difference Spectrum strategy (red), and the signal generated by our proposed model (blue).