Multi-channel Magnetic Resonance Spectroscopy GUI (McMRSGUI) User Manual

Summary: The McMRSGUI is a MATLAB-based graphical user interface that is utilized for evaluating and determining the proper multi-channel combination technique based on the spectra and additional information/scans that are available. A decision tree that is based on literature recommendations is available for the user to expedite the selection of the proper multi-channel combination between equal weighting, SNR weighting [1, 2], S/N^2 [3], WSVD [4], WSVD+Apod [4], and AOC [5]. The program currently accepts Varian, .mat, and jMRUI text files as inputs. It can likewise export data files in .mat files for recording keeping of operations performed on data, or it can be exported in a jMRUI text format for quantification with jMRUI or other 3rd party software. It provides the user with several pre-processing steps: averaging, linebroadening, zero-padding, manual 0-order and 1st-order phasing, linewidth calculation, and viewing of spectra/free induction decays.

Code Dependencies

The following are the dependencies for utilizing the MATLAB App code within Matlab:

- MATLAB: version 9.10
- Statistics and Machine Learning Toolbox: version 12.1
- Curve Fitting Toolbox: version 3.5.13

The .exe file will require MATLAB's Runtime environment [6].

Data Loading

The GUI has two main menus for loading of data: preprocessing data (Figure 1- left) and multi-channel combination (Figure 1- right). For the methods that don't account for the phasing of the spectra (equal and SNR weighting), preprocessing of data to account for 0-order and 1st-order phases is necessary. Data can be loaded in via three different formats:

1. Matlab structure with the name "Starting." The requisite fields and data types are shown in Figure 2. Note: Data is composed of free induction decay data in the matrix form (Num_channels x Num_acquisitions x Num_datapts).
2. Varian format with the .fid folder organization.
3. jMRUI TextFile format with subsequent acquisitions labeled below (Figure 3). Note: this method requires separation of channel data into different files as this format can only display multiple acquisitions.
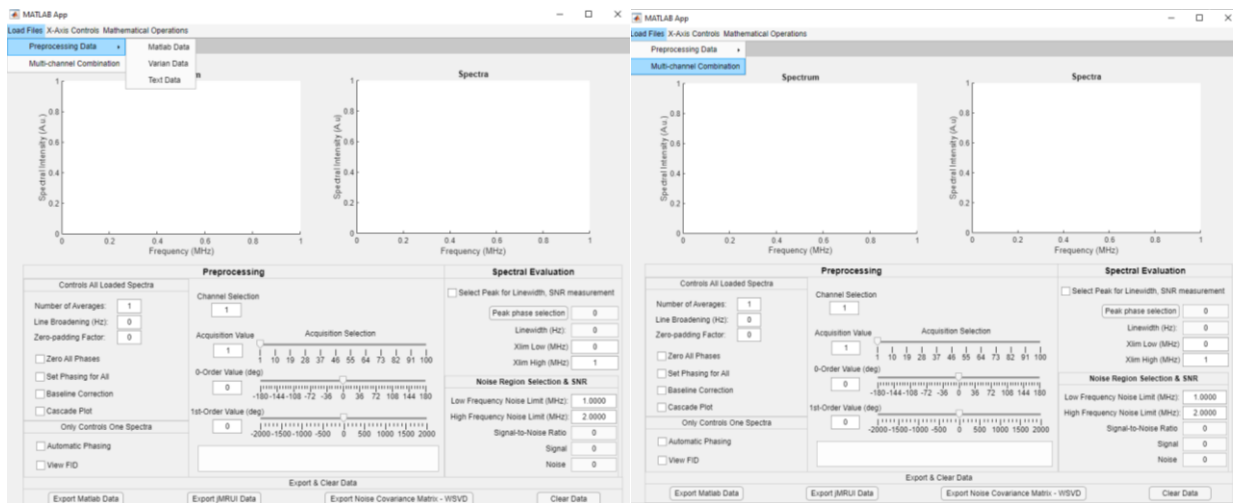
Figure 1. Data input loading options for pre-processing and multi-channel combination options.
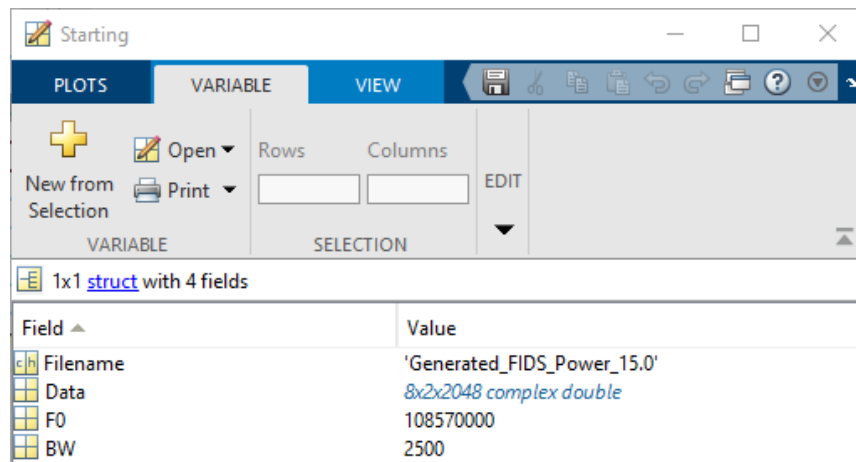

Figure 2. "Starting" structure used to initially load in data into the pre-processing menu or data-combination.

```
1    jMRUI Data Textfile
2
3    Filename: a.txt
4
5    PointsInDataset: 2048
6    DatasetsInFile: 2
7    SamplingInterval: 4.0000e-01
8    ZeroOrderPhase: 0E0
9    BeginTime: 0E0
10   TransmitterFrequency: 1.0857e+08
11   MagneticField: 0E0
12   TypeOfNucleus: -1E0
13   NameOfPatient:
14   DateOfExperiment:
15   Spectrometer:
16   AdditionalInfo:
17   SignalNames: AOC_No peak shifting combination_Acq_1;AOC_No peak shifting combination_Acq_2
18
19
20   Signal and FFT
21   sig(real)    sig(imag)   fft(real)   fft(imag)
22   Signal 1 out of 2 in file
23   4.8719e-02   1.0856e-04  4.9996e-02  -3.5887e-02
24   4.5780e-02   1.2542e-02  -5.9260e-03    -4.8040e-02
25   4.1559e-02   2.2677e-02  6.8303e-02  -6.1316e-02
26   3.2846e-02   3.0935e-02  4.9140e-03  -5.4880e-02
27   2.3149e-02   3.8705e-02  6.5260e-02  2.4192e-02
28   1.1215e-02   4.1442e-02  4.7465e-02  2.2246e-02
29   1.6106e-03   3.9560e-02  -2.0693e-02    3.8457e-02
30   -8.0924e-03  3.7110e-02  4.0934e-02  6.3387e-02
31   -1.7700e-02  3.0805e-02  4.8270e-02  -3.0141e-02
32   -2.3250e-02  2.3322e-02  3.7792e-02  1.0866e-01
33   -2.5667e-02  1.2050e-02  3.3093e-02  -8.7072e-02
34   -2.3950e-02  6.8829e-03  5.4783e-02  -2.0558e-02
35   -2.0589e-02  -2.5314e-03    4.0878e-04  -3.2301e-02
36   -1.5907e-02  -8.7015e-03    5.6513e-02  2.6439e-02
37   -7.3176e-03  -9.3210e-03    2.7653e-03  -1.2152e-02
38   -9.2471e-04  -9.4661e-03    -2.3529e-02    3.9240e-03
39   4.5122e-03   -8.5700e-03    7.7741e-02  -5.5003e-02
40   8.3108e-03   -5.2405e-03    5.7922e-02  -3.0334e-02
41   1.1310e-02   2.6805e-03  1.0950e-01  -2.6663e-02
42   1.0354e-02   8.0290e-03  5.2784e-02  1.6930e-02
43   9.4427e-03   1.3819e-02  1.5344e-01  -4.3939e-02
44   3.6808e-03   1.9484e-02  7.4505e-02  1.3286e-02
45   -6.1067e-03  2.2570e-02  2.8005e-02  3.1115e-02
46   -1.3417e-02  2.4680e-02  2.2622e-02  -3.0032e-02
47   -2.0455e-02  2.2739e-02  9.8131e-02  -9.3966e-02
48   -2.7771e-02  1.7837e-02  5.3568e-02  -2.1626e-02
```

Figure 3. jMRUI TextFile format for export option.

After the file is selected for the structure "Starting," a dialog box will appear with the total number of channels for selection. Only one channel of data can be pre-processed at a time. Following the requisite pre-processing, the processed data will need to be saved through the "Export Matlab Data" button or the batch processing menu option, shown in Figure 5. This feature allows for the manual phasing to be set and quickly iterate through each channel.
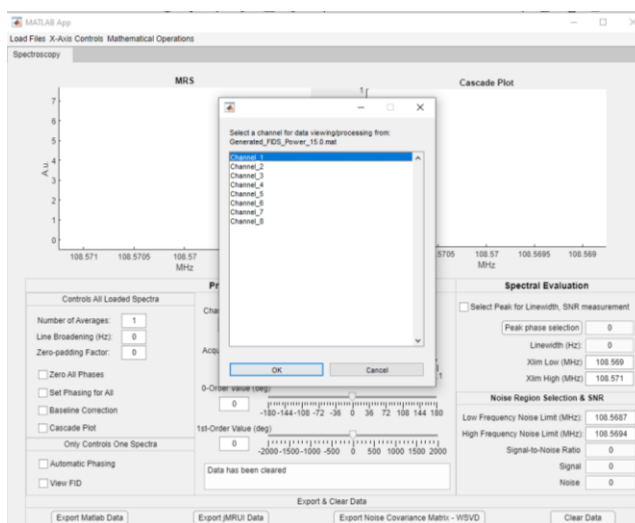

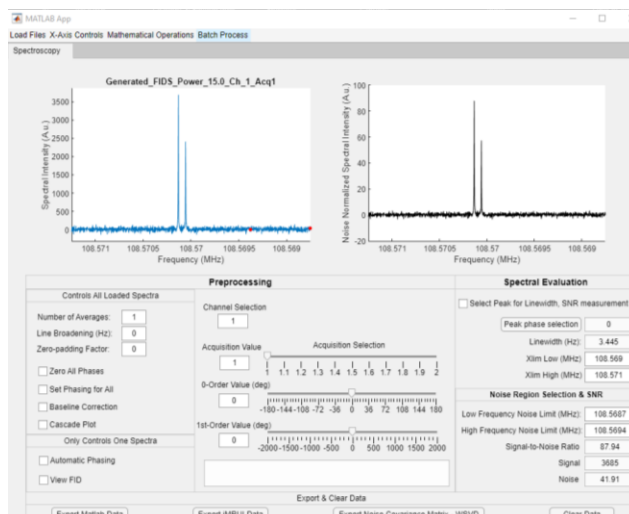*Figure 4. Individual channel selection for pre-processing.*

Figure 5. Batch Process option becomes available after data is loaded into the program and will guide the user through a short series of questions.

Pre-processing features:

1. Number of averages – for data that requires averaging of acquisitions to obtain a higher SNR. This option applies a sliding window average of length determined by the user.
2. Line broadening (Hz) – best if used for visualization purposes only, as this cuts off high frequency noise and signal content by applying a decaying exponential function to the free induction decay. A "matched-filter" or filter with the same linewidth as that of the peak of interest can be applied to evaluate the highest achievable SNR. This function is not recommended for spectral quantification.
3. Zero-padding factor – Zeros can be added to the end of the free induction decay in the time domain to interpolate datapoints in the spectral domain. This gives an increased spectral resolution from the interpolation. Data sizes can quickly become large from this.
4. Manual Phasing – Spectra can be manually phased using the bottom two sliders of Figure 5.
5. The FID for an acquisition can be viewed, or subsequent spectra can be plotted in a cascade plot for visual evaluation of trends and metabolite progression over time.
6. The peak linewidth, phase, and SNR are incorporated through the default maximum peak calculation or through user-defined regions for signal and noise.
7. The units of the x-axis can be switched between MHz and parts-per-million interchangeability for easier isolation of compounds from known chemical shifts. The options are highlighted in Figure 6.
8. File subtraction is an included feature for removing macromolecule signals or baseline roll. Note: the subtraction file must be a single acquisition (1 x Num_datapts vector).
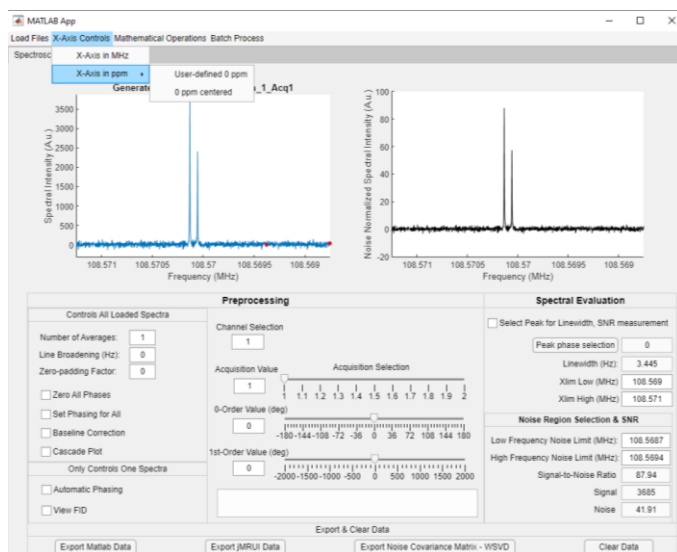
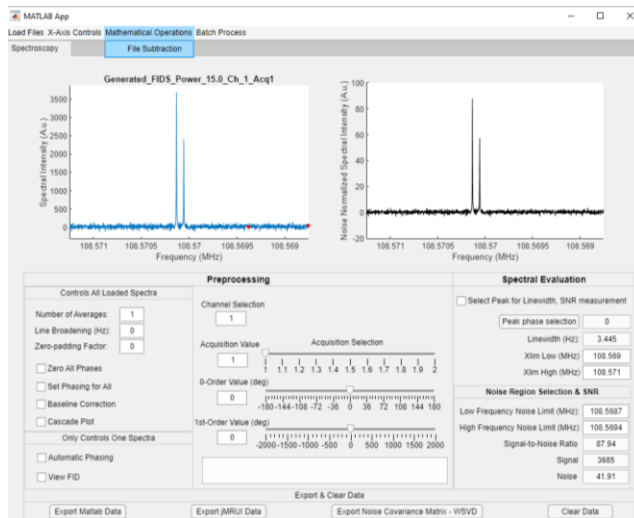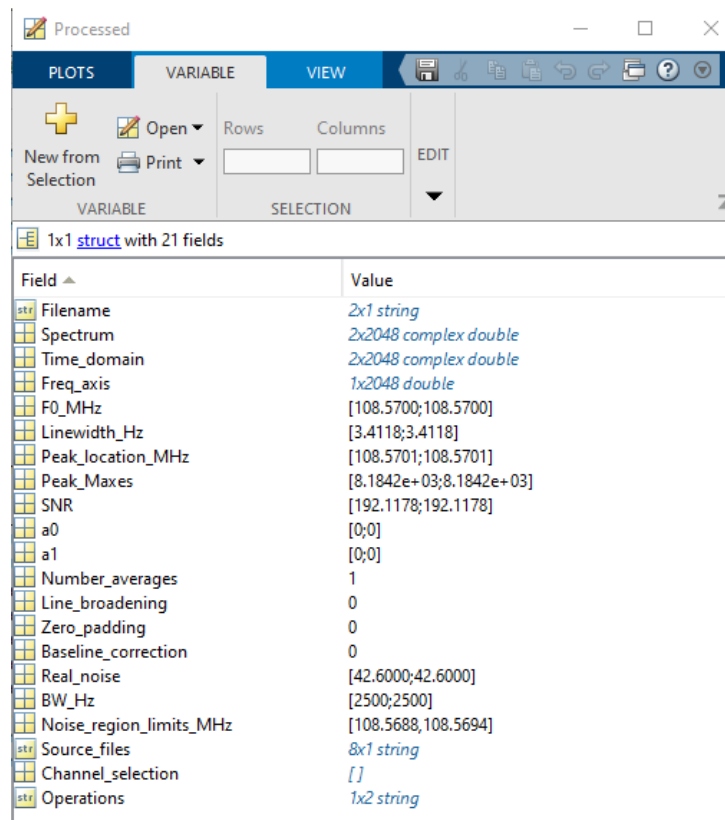Figure 6. X-axis adjustment options of MHz and parts-per-million.

Figure 7. The file subtraction function allows for a single file to be subtracted from a file to remove a macromolecule or baseline distortion.

The multi-channel combination load file's tab allows either the Matlab structure "Starting" with multi-channel data (N_channels x N_acquisitions x N_data_pts) or the Matlab structure "Processed." The additional information stored within "Processed" comes from the pre-processing step where peak information, such as the SNR and linewidth can be calculated. All other pre-processing options are stored within "Processed" to help with data traceability. The overall structure of "Processed" is shown in Figure 8. Note: If the structure "Starting" is loaded with this option, the user will be prompted for a region selection for both the noise and the signal content before the program goes back and calculates the SNR-related parameters.

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Figure 8. Processed structure information that is stored by the program.

Data Combination Tree

Following successful data loading and/or preprocessing, the multi-channel MRS data will need to be combined in a manner based on the available SNR, additional information, and noise characteristics. The program will prompt the user for a noise region that will be used for the calculation of the noise correlation. Evaluation of the data correlation levels for noise correlation between channels will help to determine if certain methods can be disregards based on their foundational assumptions. The S/N^2, S/N, and equal weighting all make the assumption that the channels are not correlated.
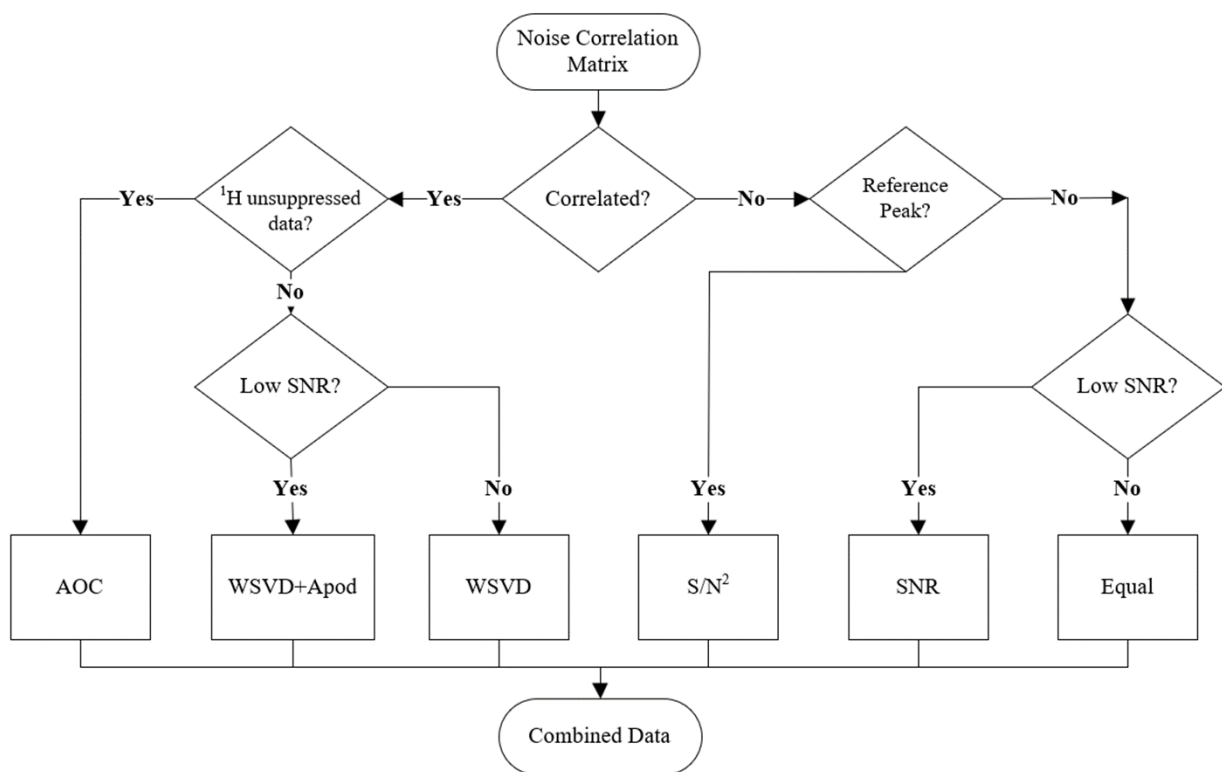
Figure 9. Multi-channel spectroscopy combination method decision tree logic utilized within the McMRSGUI.
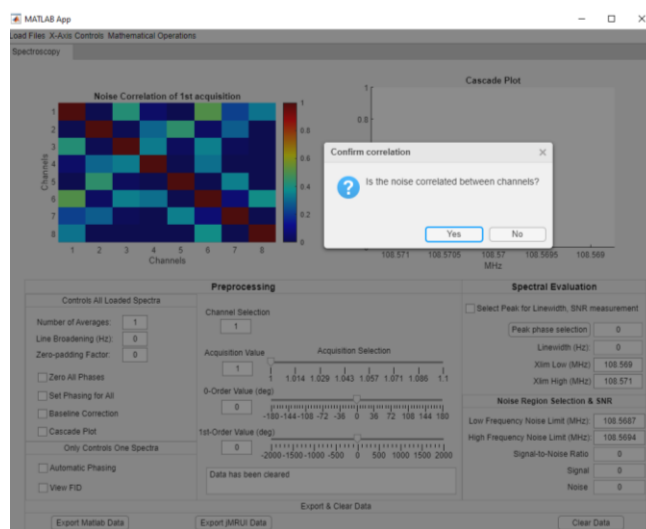

Figure 10. Decision tree for determination of noise correlation between channels.

Next, the program will prompt the user for any ^{1}H unsuppressed data scaling factors, as shown in Figure 11. The unsuppressed water peak has a high SNR and better estimates the weighting coefficients between channels. Although this is not the sole factor in determining the complex weighting factors, it does play a significant role along with the noise correlation and covariance. Methods that utilize the ^{1}H unsuppressed water scan typically better estimate the weighting factors at lower SNR when compared to their

counterparts that don't utilize it. Alternatively, a reference peak that is ever-present within the spectra can be utilized for obtaining complex weighting factors.
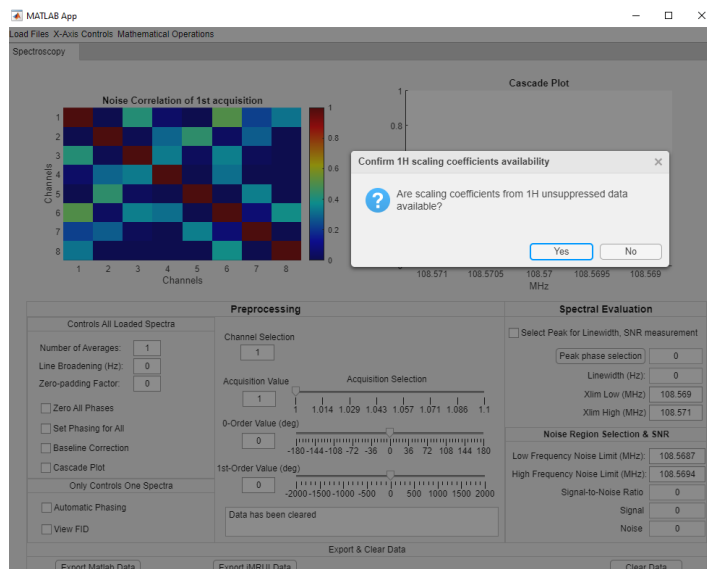

Figure 11. Question dialog for determination of 1H data availability.

The format for the ^{1}H unsuppressed data scaling factors .txt file can be found in Figure 12.
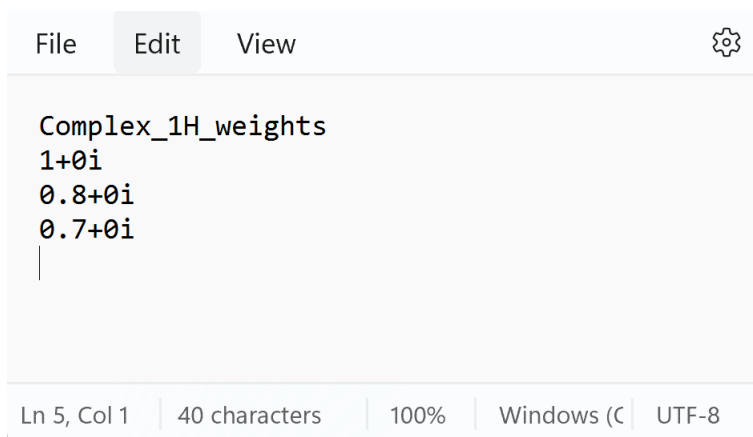

Figure 12. .txt file format for AOC complex scaling factors for a three-channel data set.

At this point, the recommended combination has either been selected or a question about whether the combined spectra is expected to be low is asked. The WSVD+Apod method performs better at lower SNR values due to the application of linebroadening for the estimation of the weighting factors. On the opposite side of the decision tree, the SNR weighting performs slightly better than the equal weighting for this scenario.

Data Exporting

As previously mentioned, the "Export Matlab Data" button, shown in Figure 13, exports a structure named "Processed." This stores all the associated pre-processing values utilized. Data that has been combined

will also be exported within "Processed" with the selection and associated additional files recorded within the structure. Alternatively, the "Export jMRUI Data" button, shown in Figure 14, will export individual acquisition data within the jMRUI Textfile format from Figure 3. This data can then be loaded in to jMRUI for quantification.
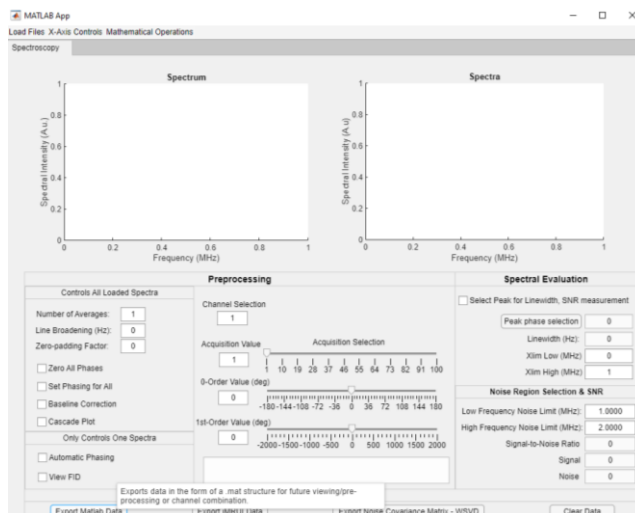

Figure 13. The "Export Matlab Data" button exports the loaded data and any associated pre-processing or combination steps for traceability.
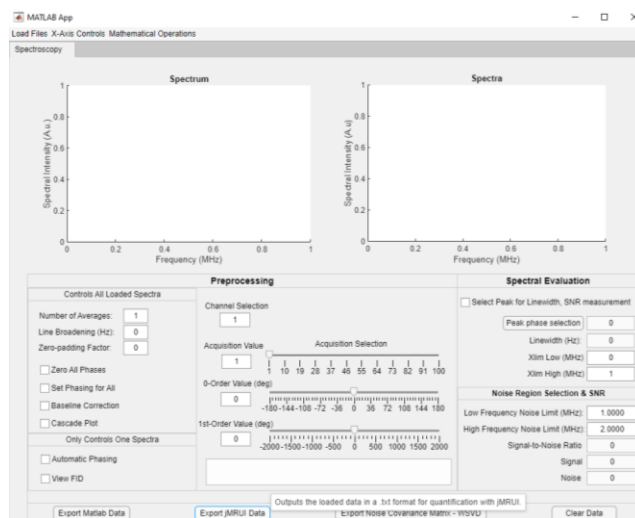

Figure 14. The "Export jMRUI Data" button exports individual acquisition data within a jMRUI Textfile format.

Resetting of the Program

To reset the GUI, the "Clear Data" button, shown in Figure 15, clears the memory of the main structure used to pass data between functions and resets the graphs.
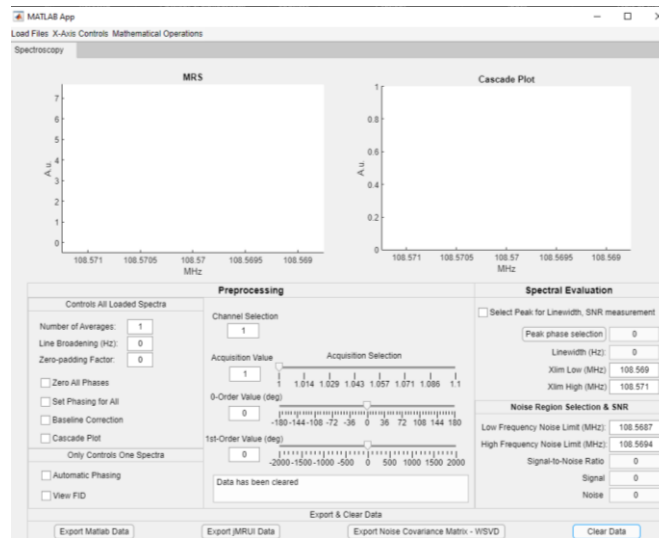
Figure 15. The clear button cleans out the information stored within the app structure.

Accompanying Programs for Simulations

1. McMRSGUI_MonteCarlo_data_simulation_creation_file.m – script utilized to create 8-channel data with correlated noise for distortion simulation. File can be modified to simulate addition channel data. The code is commented into sections with the "Inputs" that can be changed and "Calculations" for sections that shouldn't require changing. The main variables that will need to be adjusted for varied channel inputs and/or experimental full noise correlation matrices are:
   a. Num_coils – number of coils
   b. scale _factor – scaling intensity between channel data
   c. Full_noise_correlation_matrix - Num_coil x Num_coil matrix with the diagonal components representing the covariance of each channel and the off diagonal components representing the noise correlation between channels.
2. McMRSGUI_noise_covariance_creation_file.m – script that can be utilized for creating a noise covariance file for the WSVD method. An example covariance matrix produced by the code is shown in Figure 16. Alternatively, a text file (.txt) can be created with a single row of headers and then a comma-separated matrix of size Num_channel x Num_channel of the covariance values (Figure 17).

Figure 16. Example complex covariance matrix of size Num_channels x Num_channels.

Figure 17. Example covariance matrix shown in the .txt format

3. McMRSGUI_Read_jMRUI_for_S_N2_peak_amplitudes.m – script that loads in jMRUI AMARES results that were saved as a .txt file. The fitted amplitude values are then saved in the proper format for use with the McMRSGUI for the S/N^2 combination method reference peak amplitudes. An example of the weighting factors is shown in Figure 18. Alternatively, a text file (.txt) can be saved with a single row header and then a comma separated matrix of the weights (Num_channel x Num_acquisitions).

	1	2	3	4	5	6	7	8	9	10	11
1	18.0410	15.1910	14.0170	18.9510	14.2930	15.4510	17.6670	14.8530	13.1410	14.8720	12.884
2	15.7820	6.5206	10.0710	5.8835	14.6770	3.9175	8.5795	14.6590	10.1250	16.9330	16.149
3	9.8149	7.2697	10.9700	12.4720	5.7352	13.1130	7.2210	8.2904	11.6600	11.0740	11.002
4	8.5154	8.0986	13.0110	5.1433	10.4550	12.4820	5.5371	10.1850	6.8355	8.4564	11.075
5	8.1495	3.6212	10.6960	2.3340	15.3740	7.7800	7.4731	6.6382	9.6858	9.9461	5.175
6	9.6366	8.8003	13.1470	5.2931	7.0825	7.1584	11.9160	10.3030	8.5732	6.3112	11.953
7	16.9380	9.8690	18.5240	15.8350	12.9530	11.7150	16.6340	18.9690	14.6740	10.3550	12.887
8	12.7860	17.4820	17.4050	13.7380	19.5000	11.6260	19.8280	14.9040	16.3860	16.2530	15.642

Figure 18. Weighting factors for S/N2 method saved in a Num_channel x Num_acquisitions matrix.

References

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