Pantheon Parameter guide

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NOTE: Please set the paths at the beginning and ending of the code!

Magnet

This is the strength of the magnet in MHz, so typically this can be left at 400.

CSA and Aysm

These are the values of the CSA and asymmetry that you wish to simulate in a 2D experiment. If you are sim'ing a 3D experiment please see `ExcelProtonData`

Spinning_Speed

This is the spinning speed of the experiment.

Number_of_points

This is the number of points in the f1 fid of the simulated data. Note this does not have to match the experimental and in general can be left at either 96 or 120.

Crystal_file

This is the size of the crystal file. The larger the value you input the longer the experiment will take. There are more sizes that are listed in the comment in the code. If you enter an incorrect number the code will not run but it will show a list of possible numbers you can run. Tho it only works for the zcw crystal type.

Gamma_Angle

This is the number of gamma angles used in the experiment. In general the larger the better quality of the simulation but ~5 is suitable for most purposes.

DCcor

This is the number of points in the f1 sim fid that are used to lower the centre of the R16_3_2 sequence. The lower this value then the higher the middle of the spectrum becomes and vise versa. This should be set to a value so that it matches the experimental. Note this only effects R16_3_2 sequences.

Weighting_type

This is the type of line broadening that is applied. This should never be changed.

Weighting_value

This is the value of the line broadening that is applied. This simply needs to be changed to match the simulated to the experimental data.

Searchedppm

This is the ppm value that the 2D simulated data will be compared to. (if the experimental cross section does not look correct then plot a 3D version to check the ppm values of the experimental data)

Additional_Sim_Scaling

This simply scales the height of the simulated data in a 2D plot right at the end.

Spectral_Width

This is the sw of an experiment, note this only needs to be set for R16_3_2 experiments.

SimType

This can be 2D or 3D and simply decides what type of simulation is run.

MathType3DWeighting

This can be 'Gauss' or 'Matt.' This is the technique that is used for line broadening in the f2 axis for the simulated data. 'Gauss' uses a back and fourth fid weighting technique while 'Matt' uses a normal distribution technique. The difference is that 'Gauss' could be see as being slightly more 'NMR'ish but produces a artifact along the baseline. 'Matt' is done though pure maths and does not produce this baseline error.

Experiment_Type

This lets you chose which type of experiment you are going to simulate: `R16_3_2 SC212 C313`

PlotMode

This is whether you want to go 'Solo' and plot just the simulated data or to 'Compare' it to experimental data.

ExpFile

This is the file name of your experimental data. For exporting to a txt file you can type totxt in topspin. This works for `SC212 C313.` For `R16_3_2` you need to first process the experimental data in matlab before you can compare it. Please see the 'Processing R16_3_2' section for how to do that.

ExcelProtonData

This is a Excel file containing the Iso ppm, csa value and asymmetry value (in that order) for the protons you wish to simulate in a 3D spectrum. (note there must be a minimum of 3 protons)

Artifact_Removal Artifact_mid_point Artifact_Removal_width

Artifact removal smooths a window of the spectrum, where the middle of the window is the 'mid_point' and the width is the 'width.' A good tip if you wish to do this is to the run code with this off. Then you can click on the tip of the artifact to be able to obtain its X value. You then input this as the mid point and set the width to between 1-15 (depending on the experimental type) and It will remove the artifact. NOTE the width is not the width in ppm or hz but ar arbitrary scale. Between 1-15 should be used. NOTE this must be turned off for R16_3_2 experiments.

Bonus_RFinhomogeneity

This simulated additional RF inhomogeneity

Mirror_f1

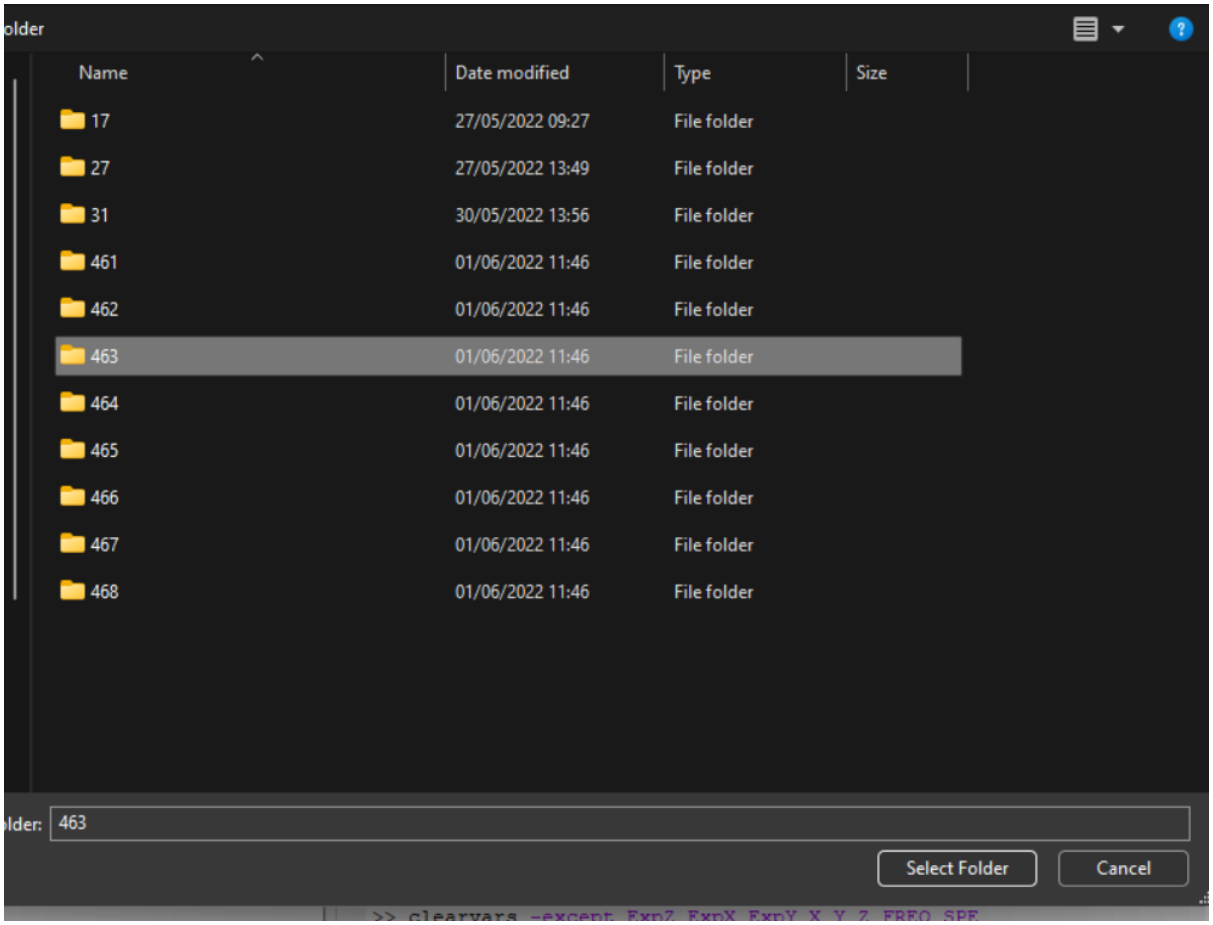
This mirrors the f1 axis in 2D simulations, does not change values simply mirrors the plotting.

Exp_2D_Hz_width

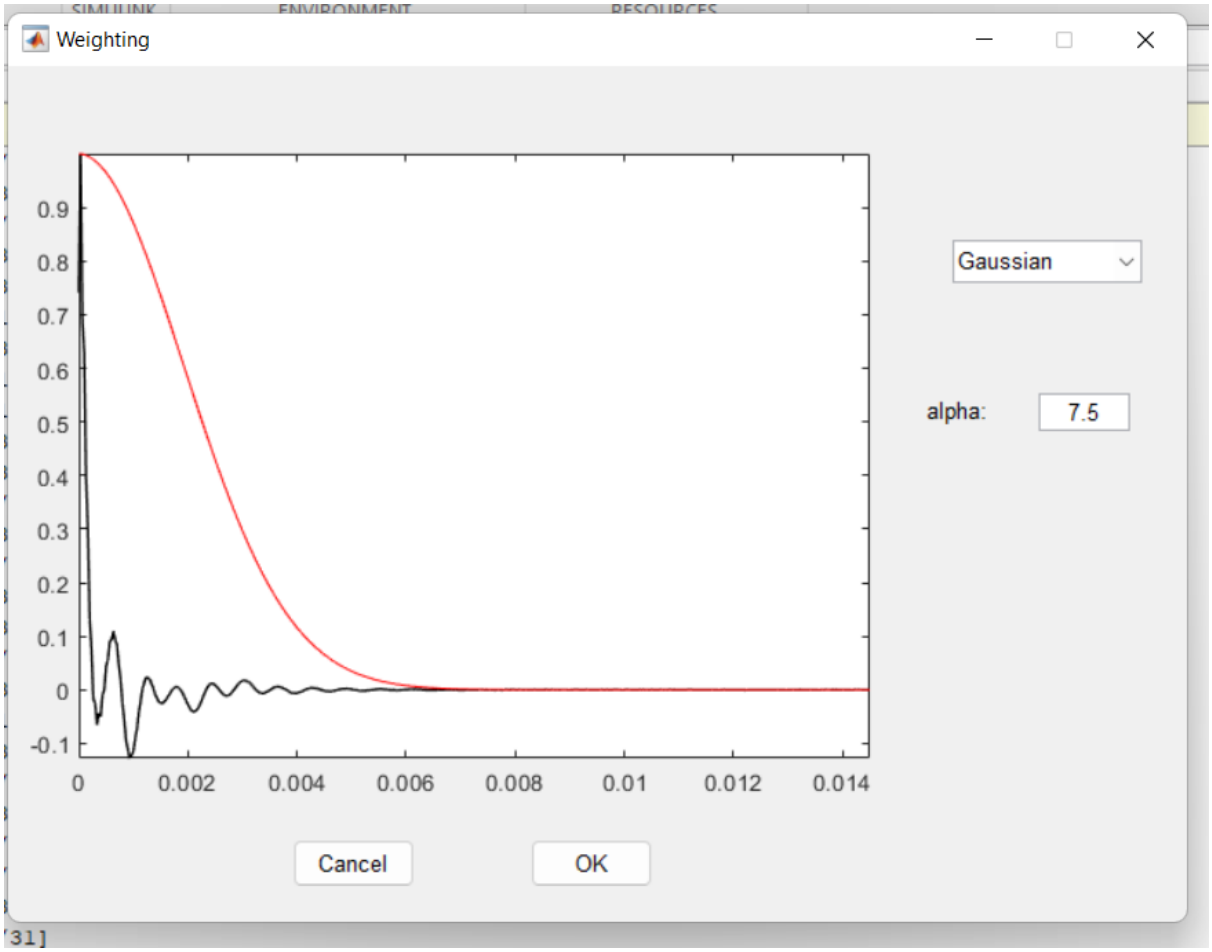
This is the width of the experiment f1 axis. Note this should be set to be ever so slightly under(could be exactly the width but if mistakenly set to big then the code will use this and mess up the plotting)

Processing R16_3_2

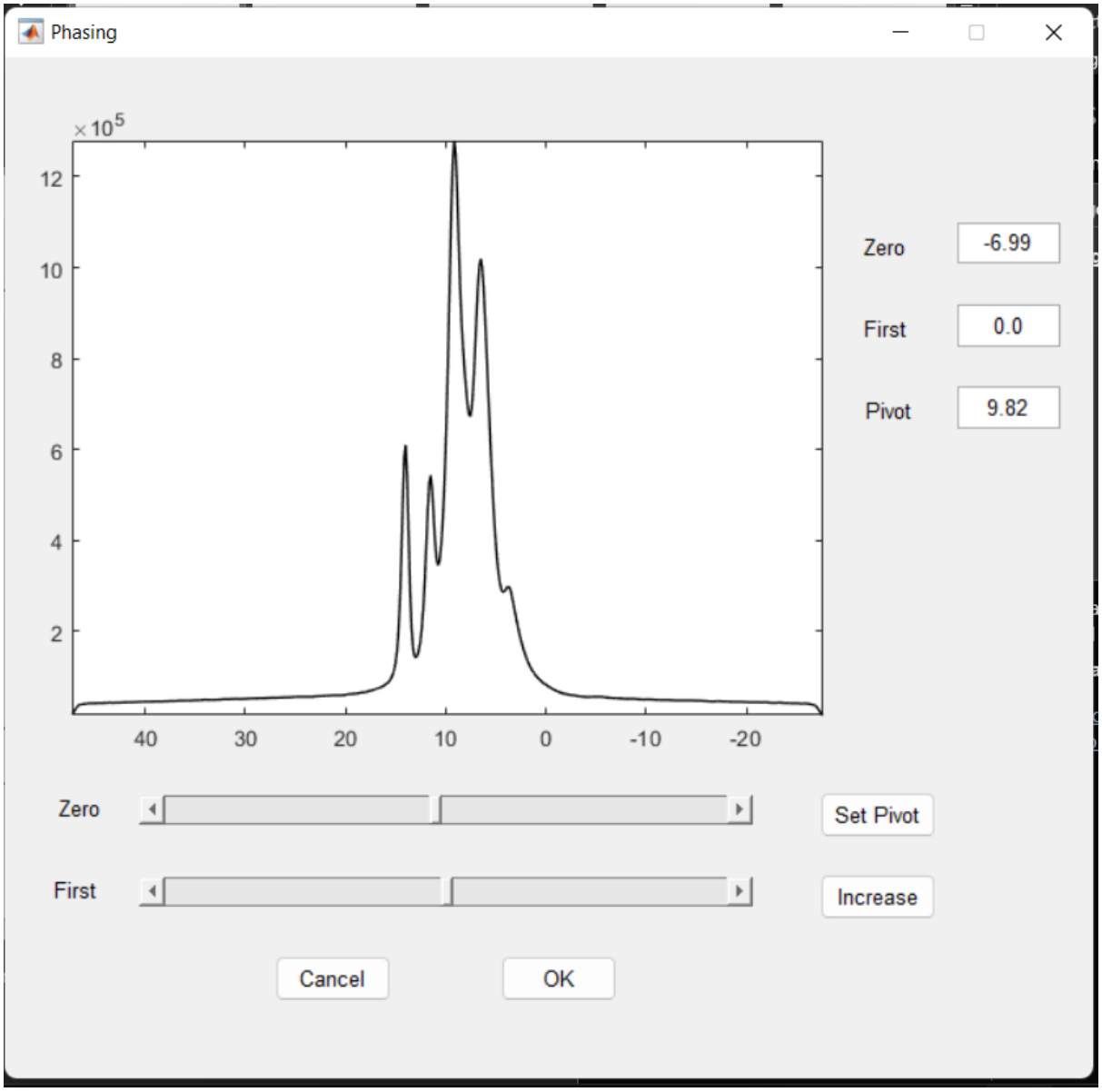
For comparing Experimental data for this sequence you should first run the code titled CSA. Initially this will lead you to a selection window.



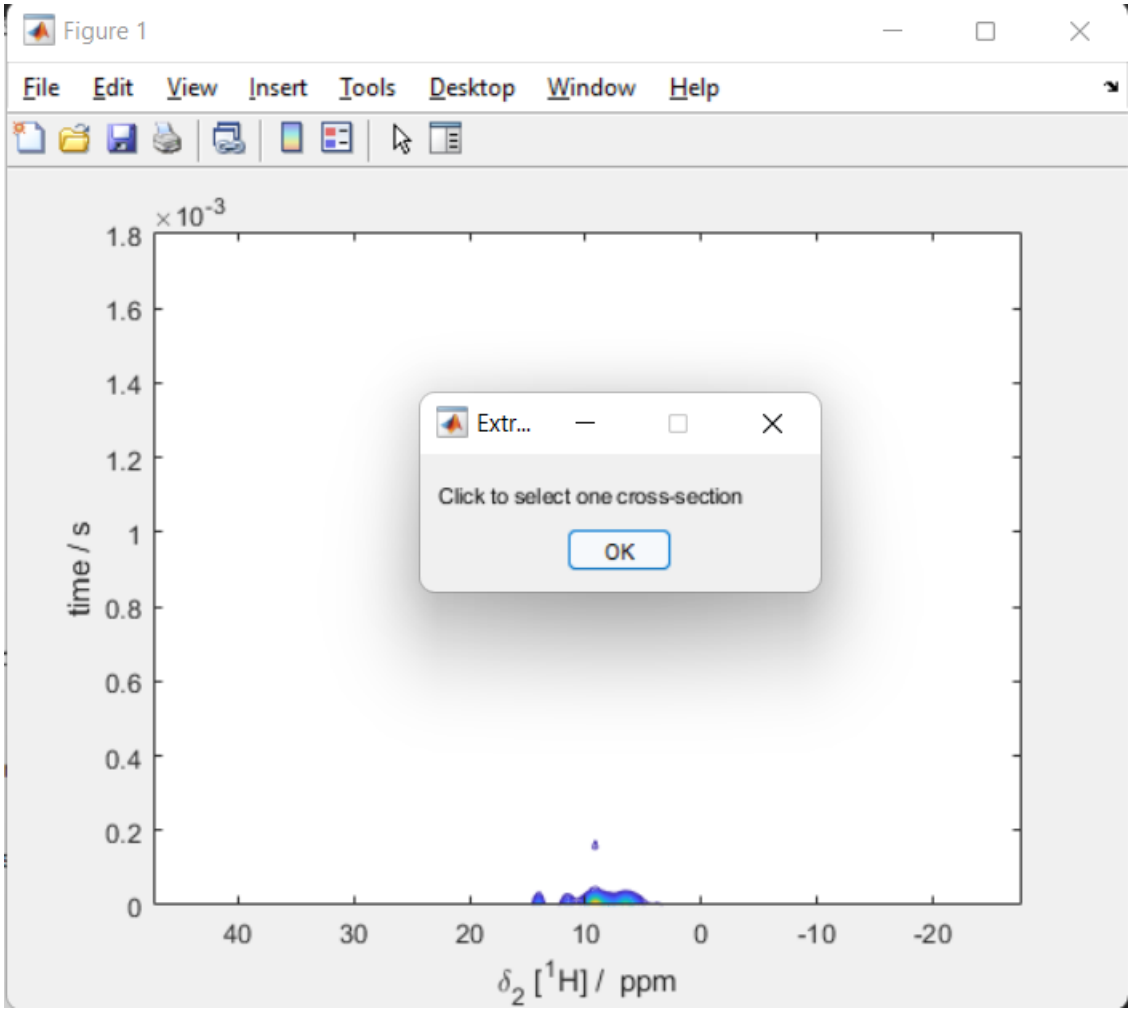
You select the folder that contains the experiment you are interested in.



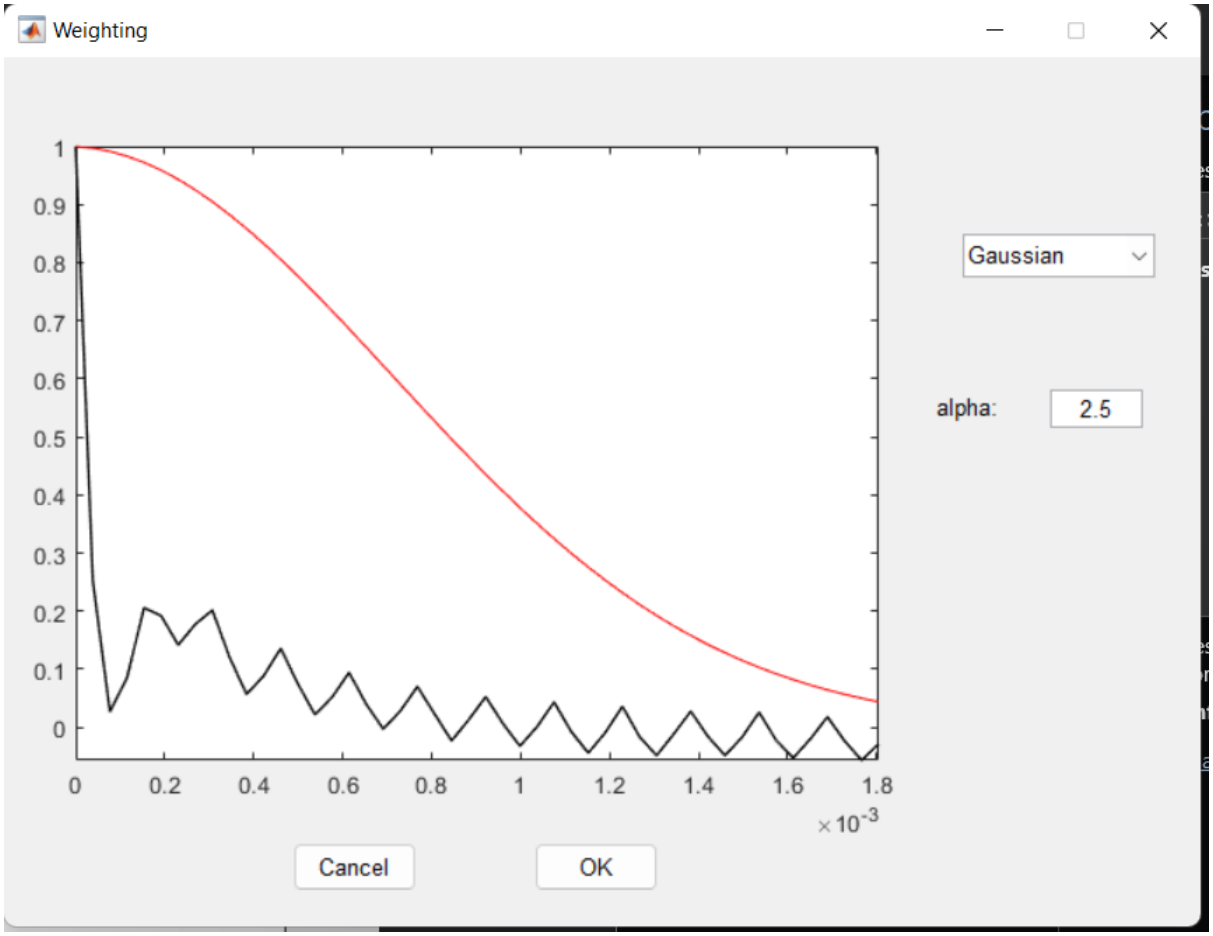
You then weight the f2 axis, a line like above is ideal as to minimise the noise but not the signal.



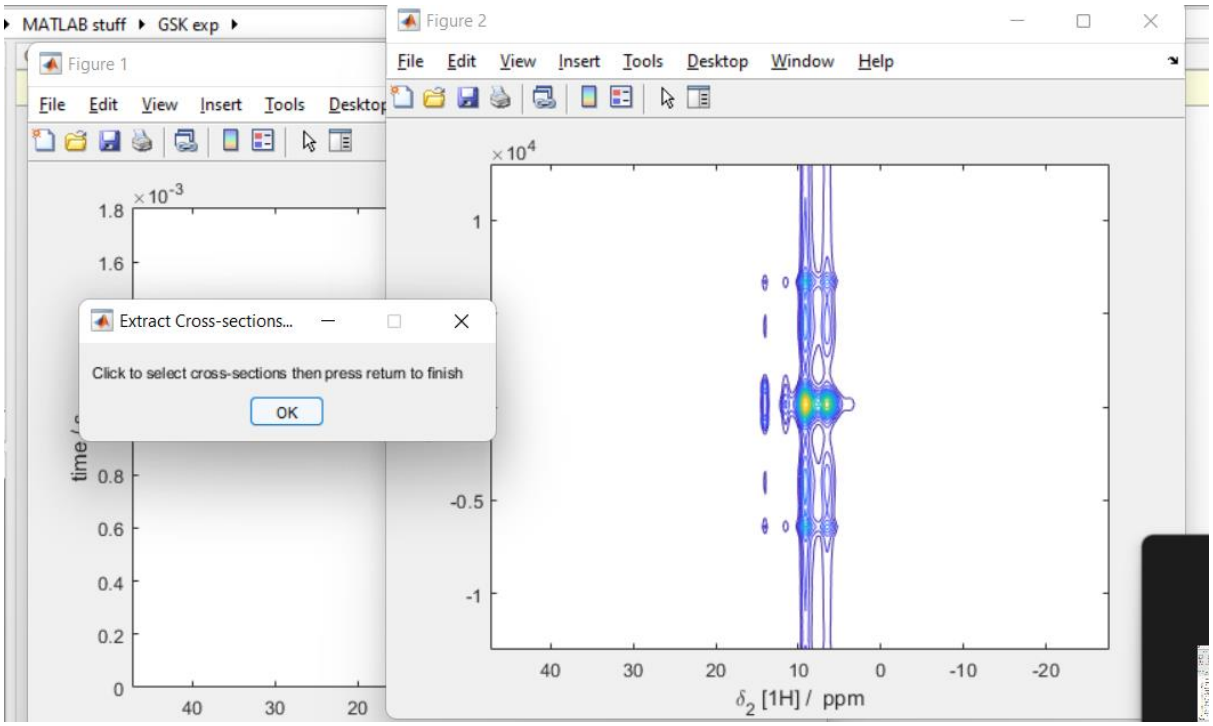
Phase the experiment in f2.



If this window pops up next click ok and click anywhere on the plot, if not ignore this sentence.

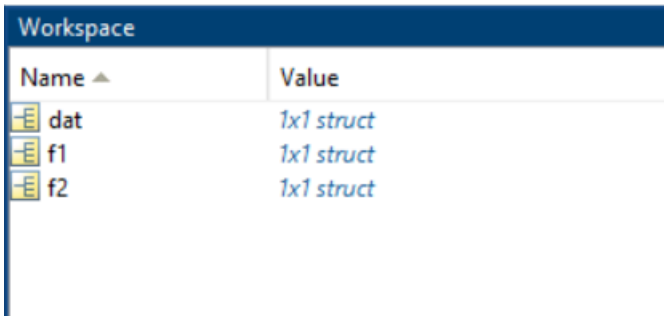


Weight the f1 axis, this should be weighted very ‘gently’ as above.



Depending on your version it will either as you to select a cross section or one will appear.

If it asks you to select the ok, click a point on the graph and hit enter. This will pop up a cross section. After this you can close down all of the graphs



In your work space you will be left with these three structures. Simply select them all and save them together as something '.mat'

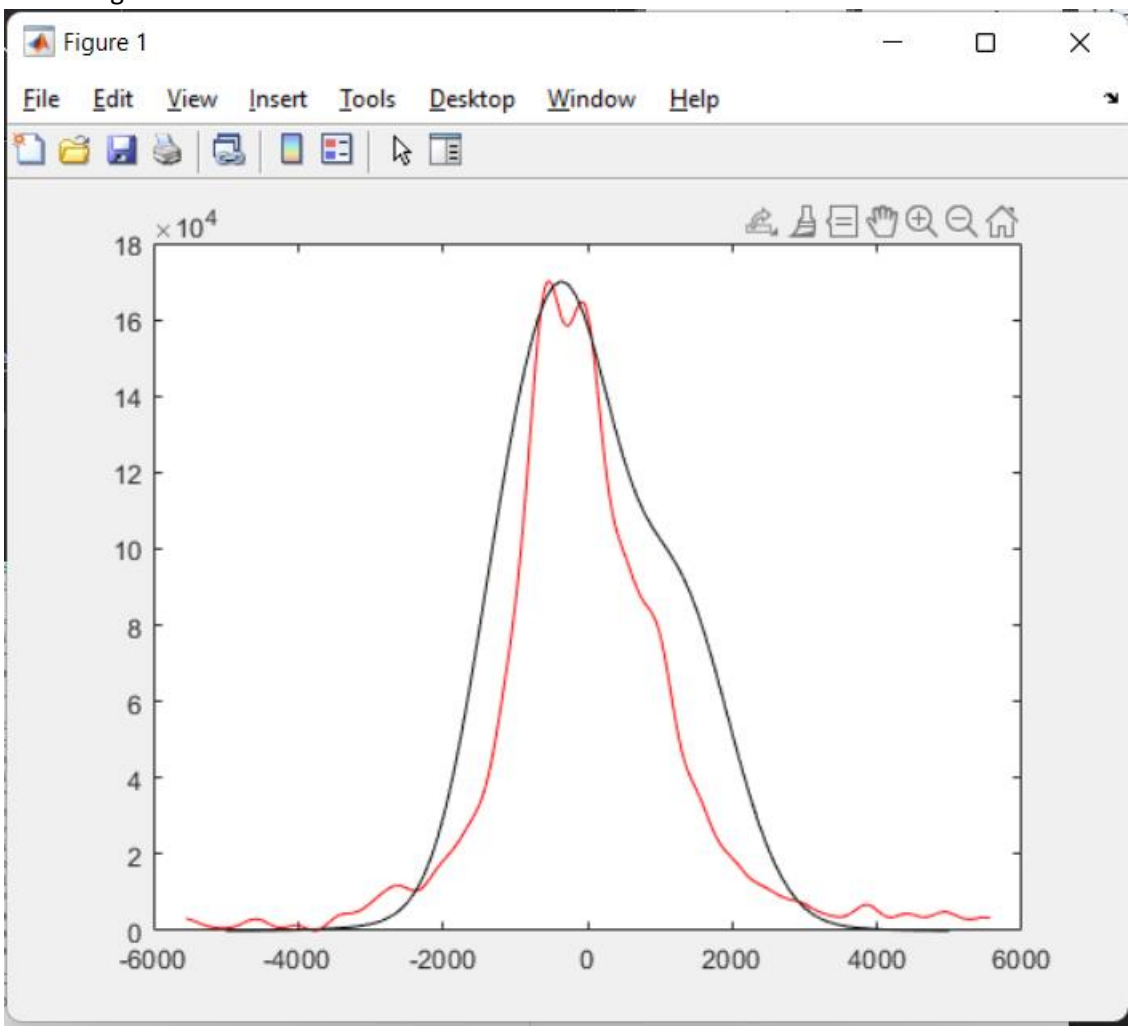
Then simply copy this to the folder containing Pantheon and past it in there. This can then be used instead of a .txt file for `ExpFile` while doing `R16_3_2` experiments.

Example: Performing a 2D simulation of SC212 at 20ppm for CSA and 0.5 for asymmetry and comparing it the an experimetnal proton at 12ppm.

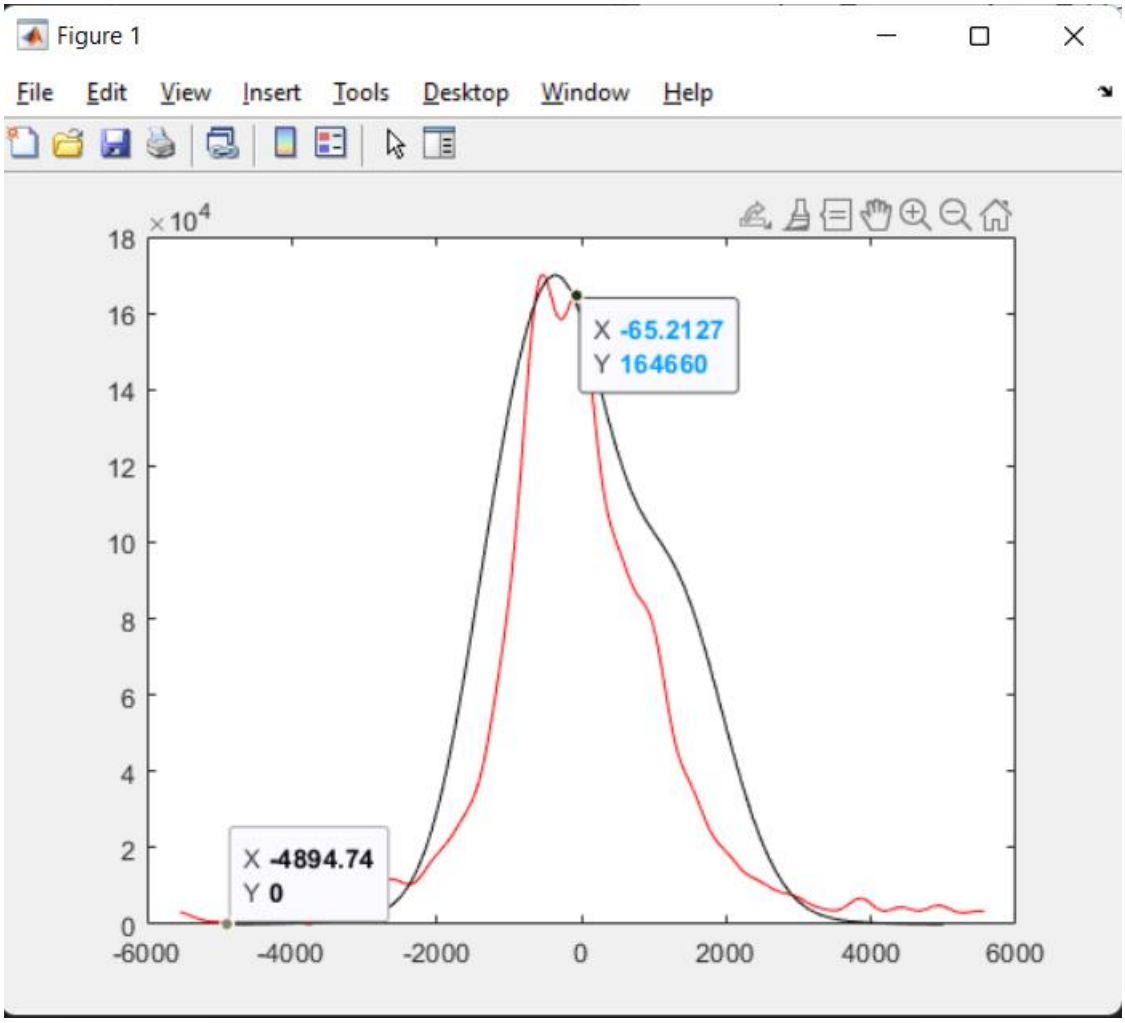
```
%% Settable Parameters
Magnet = 400;                    % Magnet strength in MHz
CSA = 20;                        % 2D simulated Chemical Shift Anisotropy value
Aysm = 0.5;                      % 2D simulated Asymmetry
Spinning_Speed = 40000;          % 2D or 3D simulation spinning speed
Number_of_points = 96;           % Number of points in the f1 dimension of simulation
Crystal_file = 20;              % Crystal file number. Typically use 20, 143, 232, 615 NOTE  takes longer
Gamma_Angle = 5;                 % Number of angles tested. ~5-10 for quick analysis,  ~32 for high quality NOTE  takes longer
DCcor = 46;                      % Number points of the FID that are averaged to bring the dipole-dipole coulping down.
Weighting_type = 'Gaussian';     % Type of weighting parameter
Weighting_value = 30;           % 'Power' of the above weighting type
Searchedppm = 12;                % The ppm value that the '2D' data will compare itself to.
Additional_Sim_Scaling = 1;      % Used to bring down peak heights to combat artifact
Spectral_Width = 26041;          % Only needs to be set for R16_3_2
SimType = '2D';                  % 2D or 3D
MathType3DWeighting = 'Gauss';   % Gauss or Matt
Experiment_Type = 'SC212';        % Currently Available: R16_3_2 SC212 C313
PlotMode = 'Compare';            % Solo or Compare
ExpFile = 'SC212.txt';            % Name of the bruker txt file(must be 2D) or processed .mat file for R16_3_2
ExcelProtonData = 'csatest.xlsx'; % Name of the excel file containing the CASTEP data (column 1: Iso, column 2: Aniso, column 3: Aysmmetry)
Artifact_Removal = 'Off';         % Removes the artifact at 0Hz in experimental data
Artifact_mid_point = -104;          % Moves the Artifact removal window
Artifact_Removal_width = 4;      %Sets the size of the removal window
Bonus_RFinhomogeneity = 'Off';   % Uses a larger profile for rf inhomogeneity. NOTE  takes longer
Mirror_f1 = 'Off';               % Reverses the f1 axis
Exp_2D_Hz_width = 12000;           % Width of F1 in Hz (only affected when artifact removal is on)

```

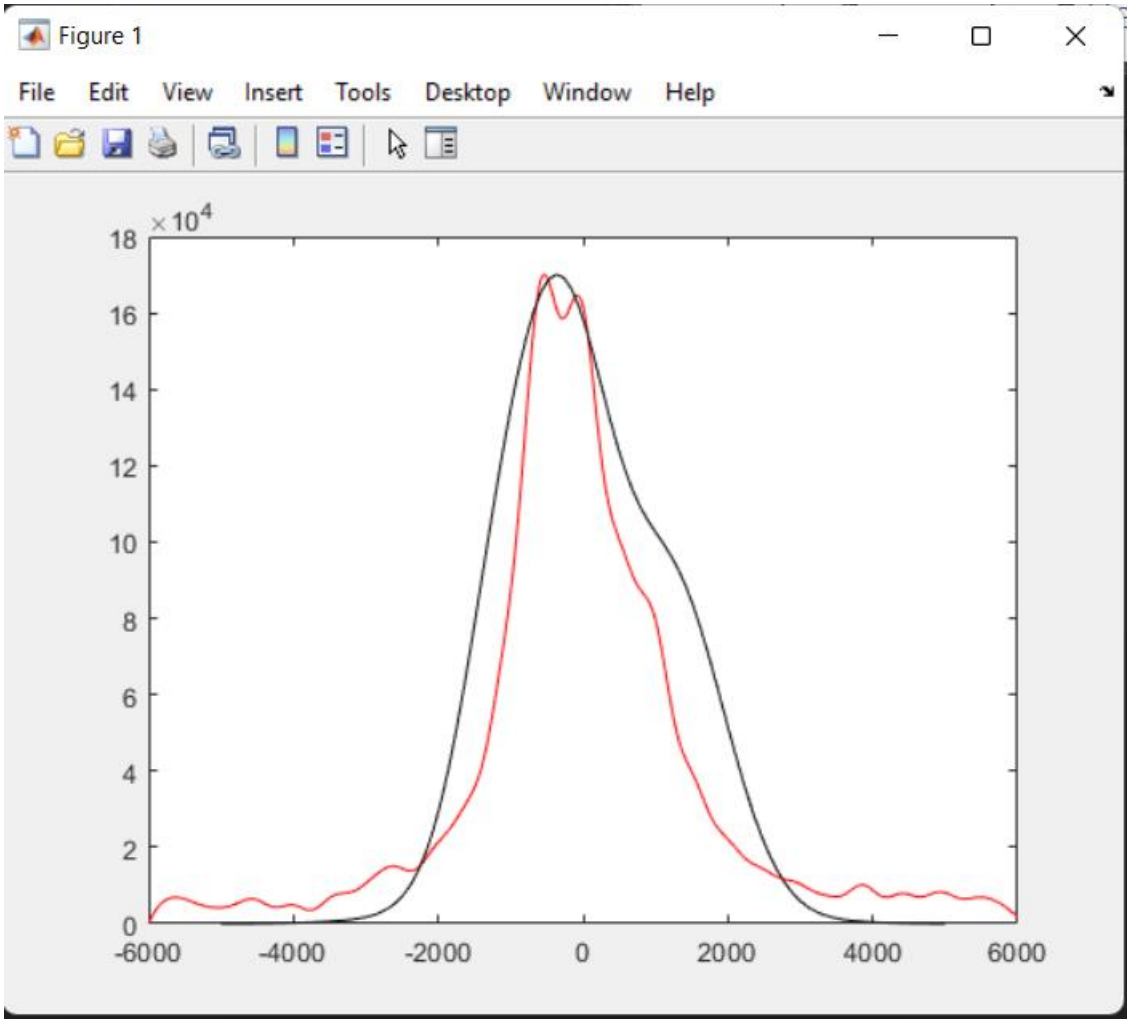
Producing



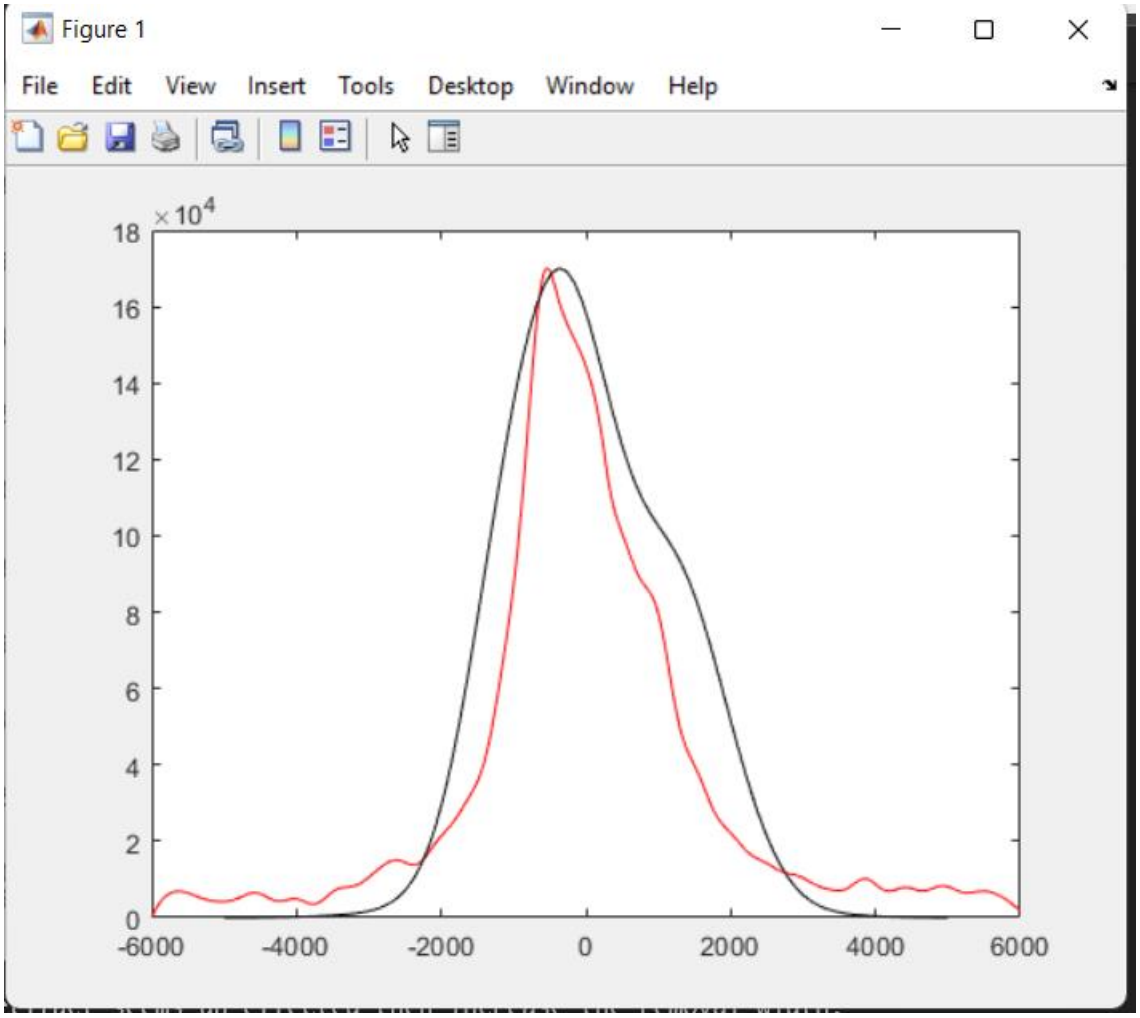
Removing the artifact for help calculating the CSA.



Find the X value of the artifact by clicking it. Then set `Artifact_mid_point = -65;`



If the artifact seems un effected then increase the removal width.

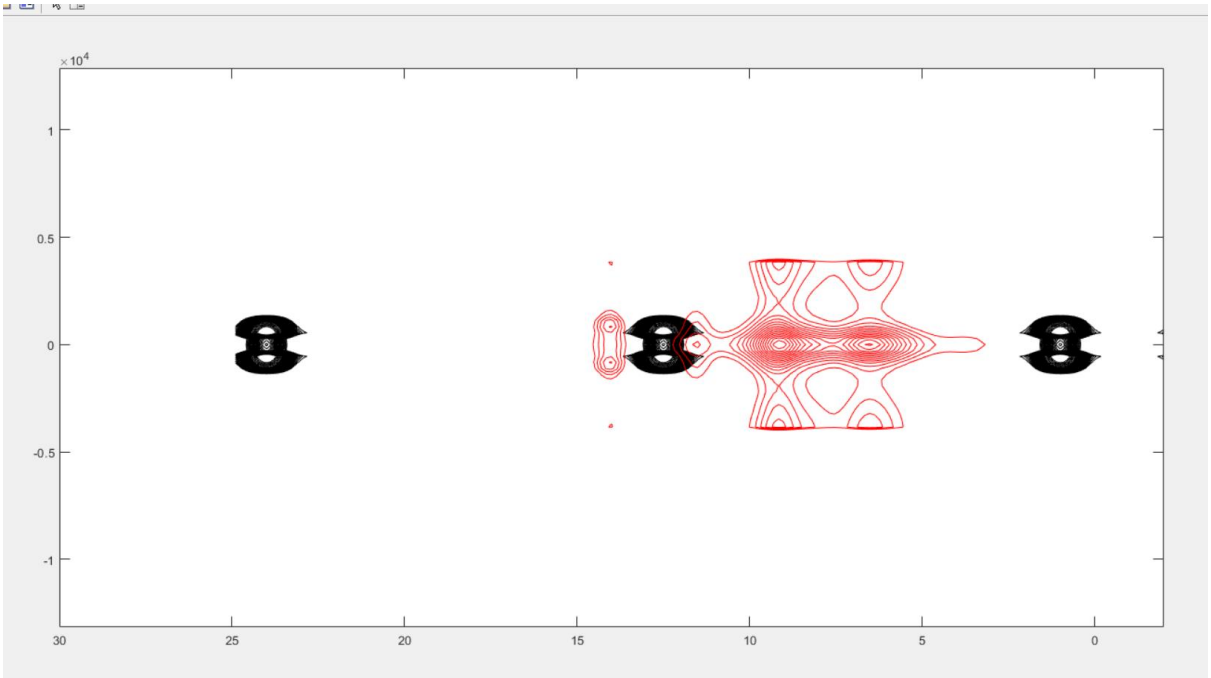


In this case going to 15 was enough.

Example: Comparing a 3D simulation of data to experiment data in an R16_3_2 experiment.

The csatext.xlsx is used for this. This contains 3 protons that are evenly spaced throughout the typical proton ppm range.

```
%% Settable Parameters
Magnet = 400;                       % Magnet strength in MHz
CSA = 20;                           % 2D simulated Chemical Shift Anisotropy value
Aysm = 0.5;                         % 2D simulated Asymmetry
Spinning_Speed = 58600;             % 2D or 3D simulation spinning speed
Number_of_points = 96;              % Number of points in the f1 dimension of simulation
Crystal_file = 20;                 % Crystal file number. Typically use 20, 143, 232, 615 NOTE  takes longer
Gamma_Angle = 5;                    % Number of angles tested. ~5-10 for quick analysis,  ~32 for high quality NOTE  takes longer
DCcor = 46;                         % Number points of the FID that are averaged to bring the dipole-dipole coulping down.
Weighting_type = 'Gaussian';        % Type of weighting parameter
Weighting_value = 2.5;              % 'Power' of the above weighting type
Searchedppm = 12;                   % The ppm value that the '2D' data will compare itself to.
Additional_Sim_Scaling = 1;         % Used to bring down peak heights to combat artifact
Spectral_Width = 26041;             % Only needs to be set for R16_3_2
SimType = '3D';                     % 2D or 3D
MathType3DWeighting = 'Gauss';      % Gauss or Matt
Experiment_Type = 'R16_3_2';           % Currently Available: R16_3_2 SC212 C313
PlotMode = 'Compare';               % Solo or Compare
ExpFile = 'tyrosineEXP.mat';              % Name of the bruker txt file(must be 2D) or processed .mat file for R16_3_2
ExcelProtonData = 'csatest.xlsx'; % Name of the excel file containing the CASTEP data (column 1: Iso, column 2: Aniso, column 3: Aysmmetry)
Artifact_Removal = 'Off';            % Removes the artifact at 0Hz in experimental data
Artifact_mid_point = -65;             % Moves the Artifact removal window
Artifact_Removal_width = 15;         %Sets the size of the removal window
Bonus_RFinhomogeneity = 'Off';      % Uses a larger profile for rf inhomogeneity. NOTE  takes longer
Mirror_f1 = 'Off';                  % Reverses the f1 axis
Exp_2D_Hz_width = 12000;               % Width of F1 in Hz (only affected when artifact removal is on)
```

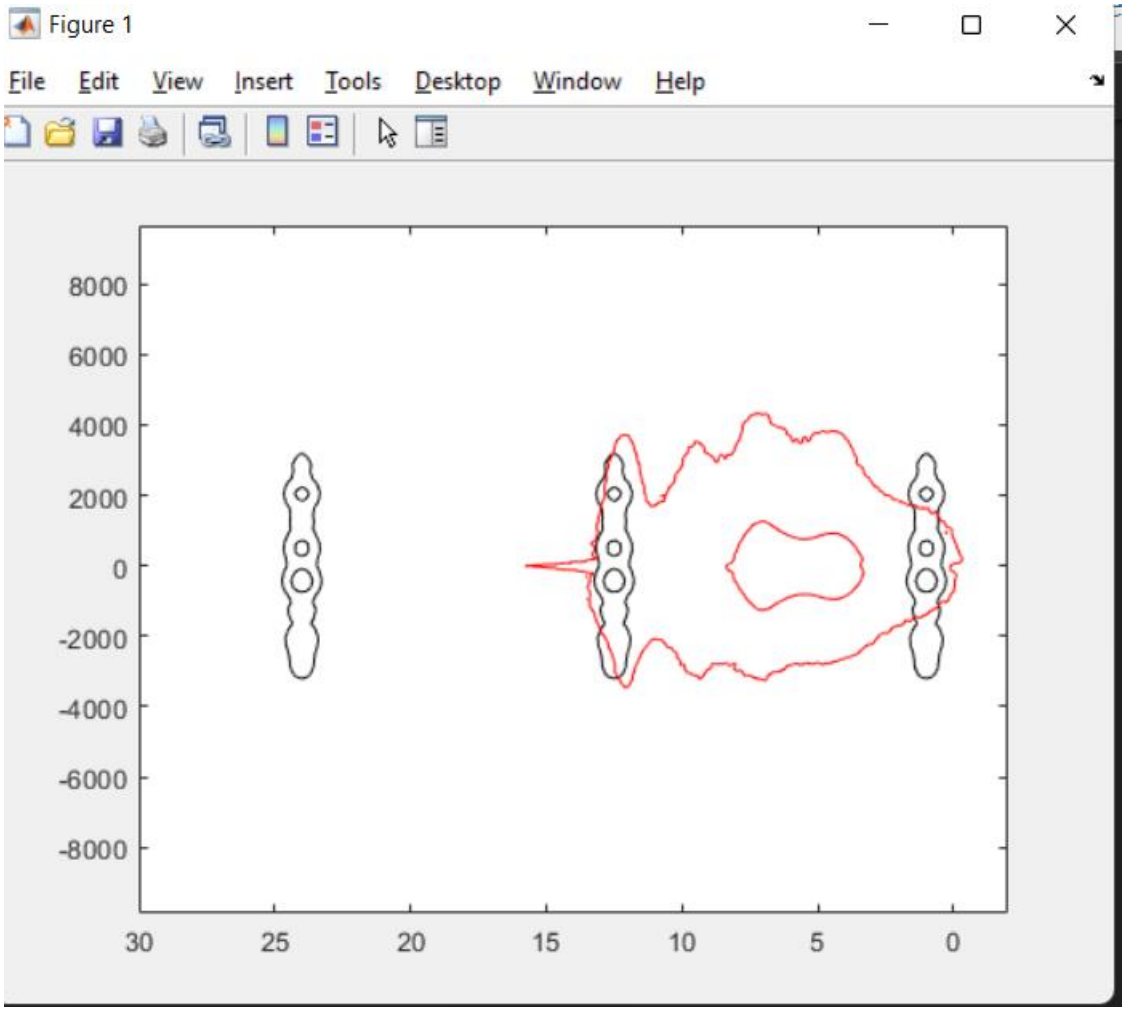


If we wanted to decrease the amount of noise that shows we can decrease the number of contours that are seen we can quickly change this using the ‘QuickPlot’ code.

```
%% Plotting Parameters
Additional_Sim_Scaling = 1;
SimType = '3D'; %2D or 3D
PlotMode = 'Compare'; %Solo or Compare
switch SimType
    case '2D'
        SPE = SPE*Additional_Sim_Scaling;
        switch PlotMode
            case 'Compare'
                plot(ExpX,ExpY, 'color', 'r')
                hold on
                plot(FREQ,SPE, 'color', 'k')
            case 'Solo'
                plot(FREQ,SPE, 'color', 'k')
        end
    case '3D'
        switch PlotMode
            case 'Compare'
                %% Plots Sim data
                pl=[1.0,0.9,0.75,0.6,0.5,0.45,0.4,0.35,0.325,0.3,0.275,0.25,0.24,0.23,0.22,0.21,0.2,0.19,0.18,0.17]; % default contour levels
                pl=pl*max(max(Z));
                contour(X,Y,Z,pl,'k');
                hold on
                %% Plots Experimental data
                pl=[1.0,0.9,0.75,0.6,0.5,0.45,0.4,0.35,0.325,0.3,0.275,0.25,0.24,0.23,0.22,0.21,0.2,0.19,0.18,0.17];
                pl=pl*max(max(real(ExpZ)));
                contour(ExpX,ExpY,ExpZ,pl,'r')
                set(gca, 'XDir','reverse') %reverse x axis
                xlim([-2 30])
                hold off
            case 'Solo'
                pl=[1.0,0.9,0.75,0.6,0.5,0.45,0.4,0.35,0.3,0.25,0.2];
                pl=pl*max(max(Z));
                contour(X,Y,Z,pl,'k');
                set(gca, 'XDir','reverse') %reverse x axis
        end
end
```

The pl are the contour levels that show for the Sim and experiment data and these can be changed to whatever you want.

For example setting both to pl=[1.0,0.5,0.1];



we get this ugly monster.

Easy_Pantheon