



MRS4brain Toolbox

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Version 0.1, November 2023



0 - MODALITIES



Menu MRSI SVS DWS

  **MRS4BRAIN Toolbox**

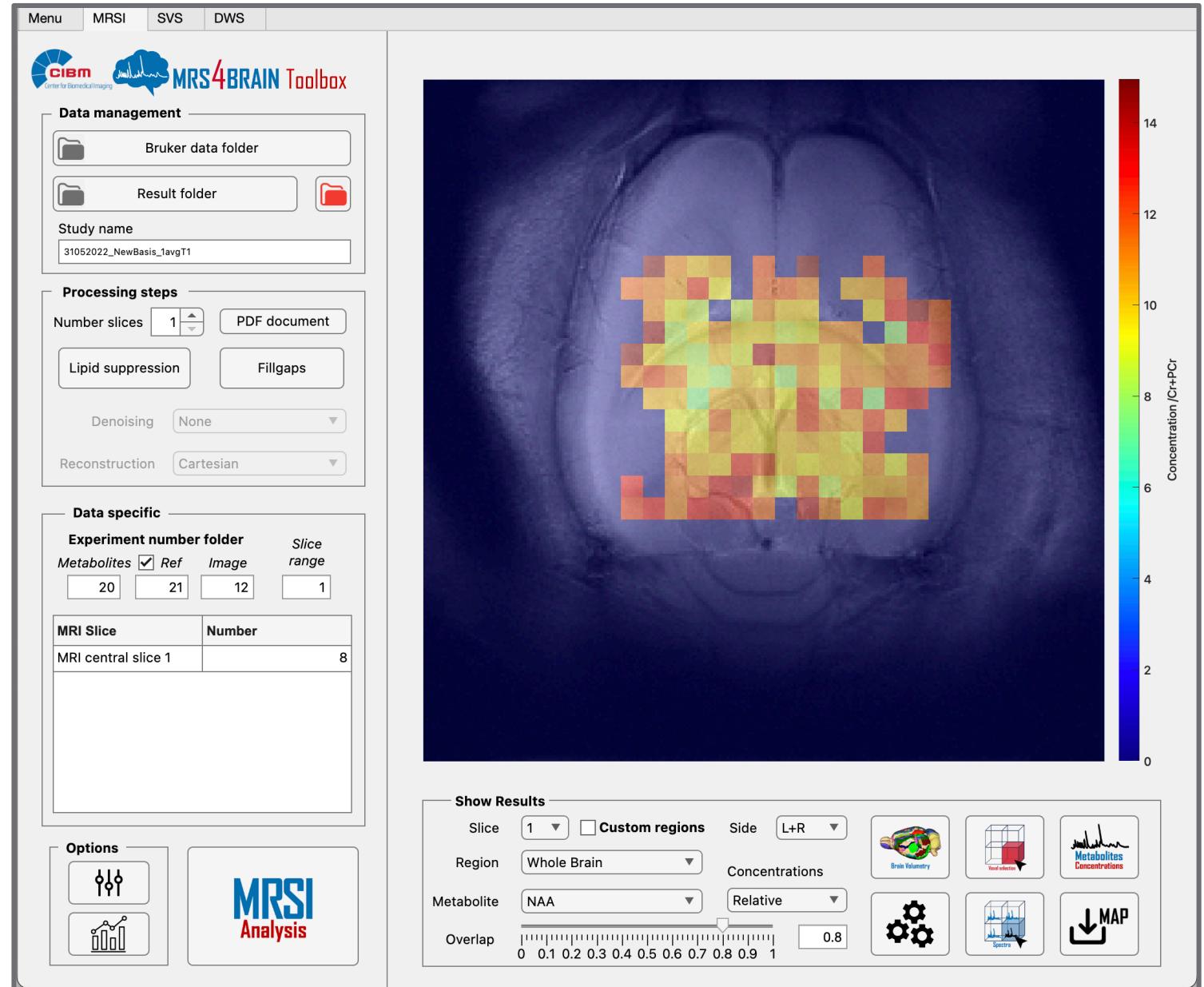
Welcome to the MRS4Brain Toolbox, Please select one of the following spectroscopy modalities

Magnetic resonance spectroscopic imaging 

Single voxel spectroscopy 

Diffusion weighted spectroscopy 

1 - MRSI



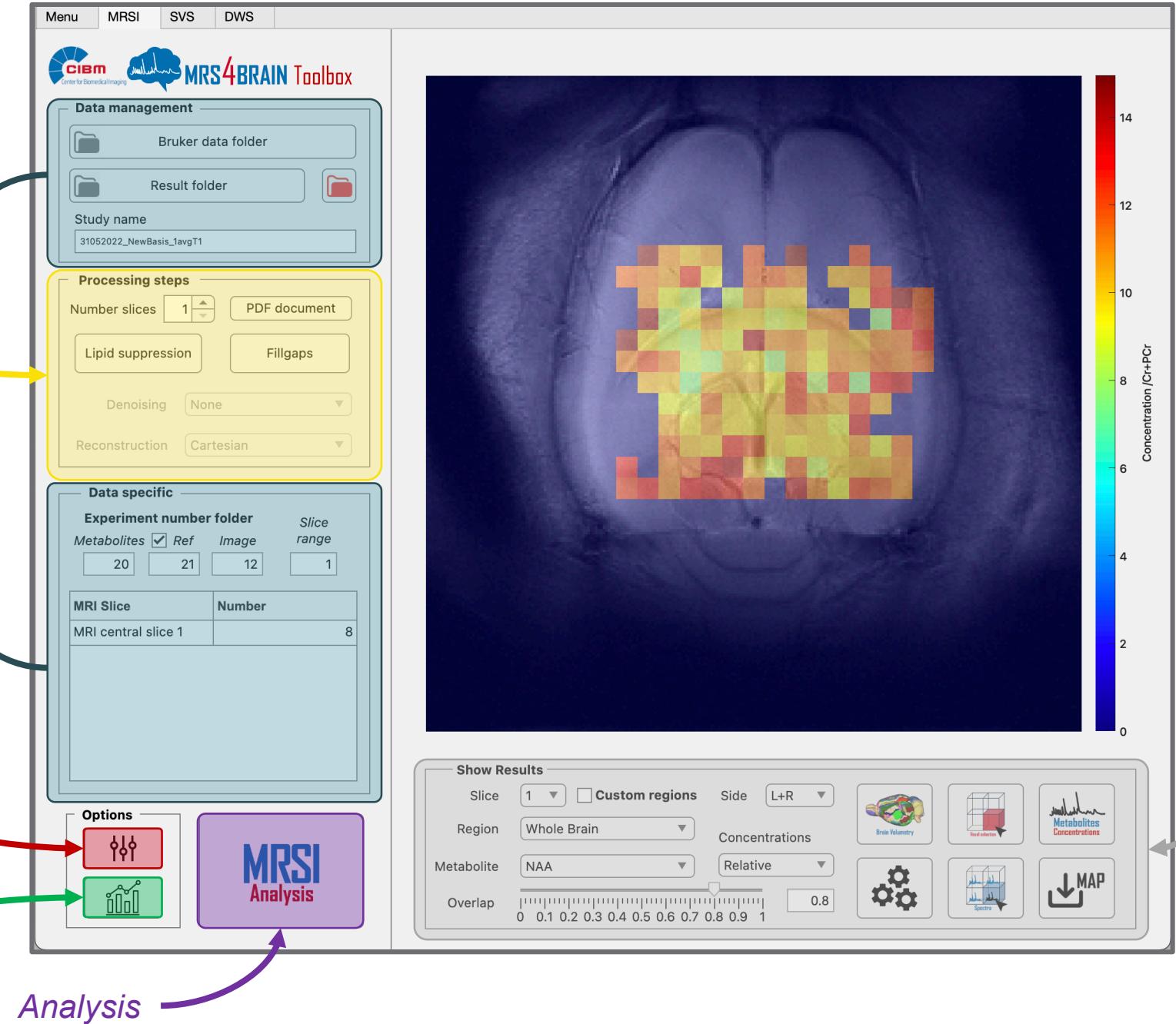
1 - MRSI

Preprocessing steps

Bruker data management

*Parameters
(Fitting, registration)*

Statistics



1 - MRSI BRUKER Data Management

Data management

Bruker data folder	
Result folder	
Study name	31052022_NewBasis_1avgT1

1.2

1.1

1.3

1.4

Data specific			
Experiment number folder			
Metabolites	<input checked="" type="checkbox"/> Ref	Image	Slice range
20	21	12	1
MRI Slice	Number		
MRI central slice 1	8		

1.1. Selection of a Bruker data folder

1.2. Selection of a result folder (where the study will be saved)

1.3. Selection of a study folder

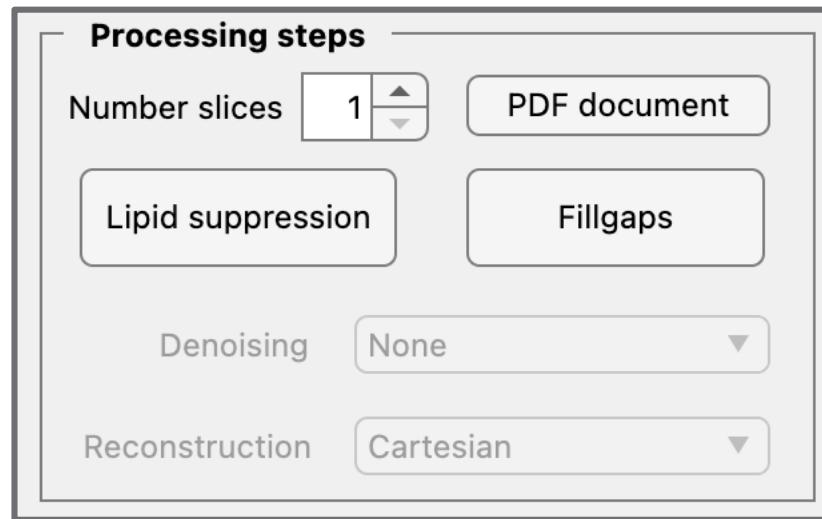
1.4. Name of the study - where the results will be saved

2.1. Bruker experiment number for metabolite, reference and MRI image acquisition (WIP : reference image can be omitted)

2.2. Number of MRI slices needed to form an MRSI slab

2.3. MRI central slice for each MRSI slab studied

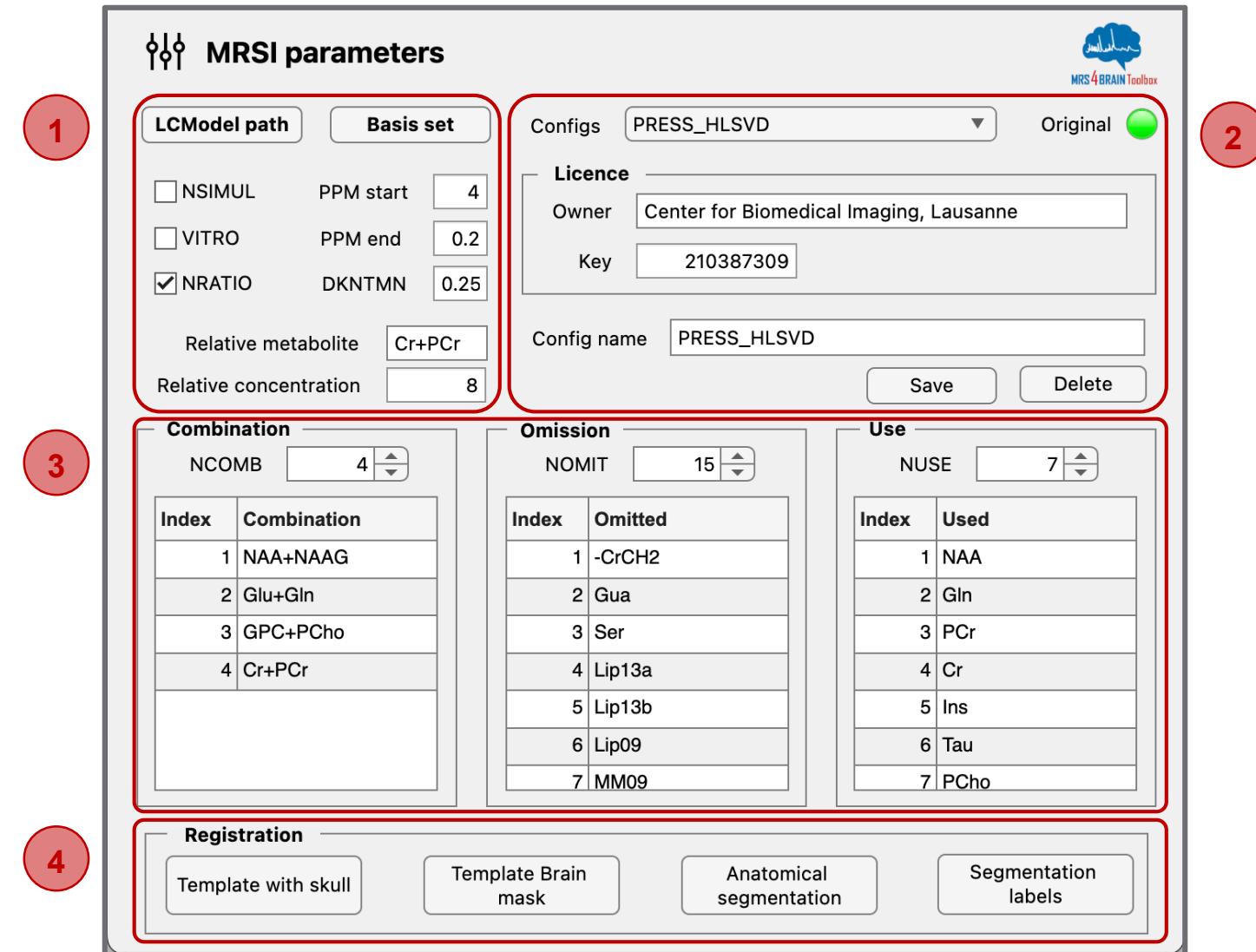
1 - MRSI Preprocessing steps



1 2 3 4 5 6

1. Number of MRSI slices/slab studied
2. PDF document : Open the Bruker data folder and allow user to open a PDF document to look at an experiment sheet with exp numbers
3. Lipid suppression technique using SVD and L2 regularisation, works on 1H-FID-MRSI data
4. WIP : Fillgaps method to recover the free induction decay data points limited by the acquisition delay (AD)
5. WIP : Denoising techniques (MP-PCA, LR-TGV)
6. WIP : Cartesian and non cartesian reconstruction techniques

1 - MRSI Parameters (Fitting, registration)



The screenshot shows the 'MRSI parameters' configuration window. The interface is divided into several sections:

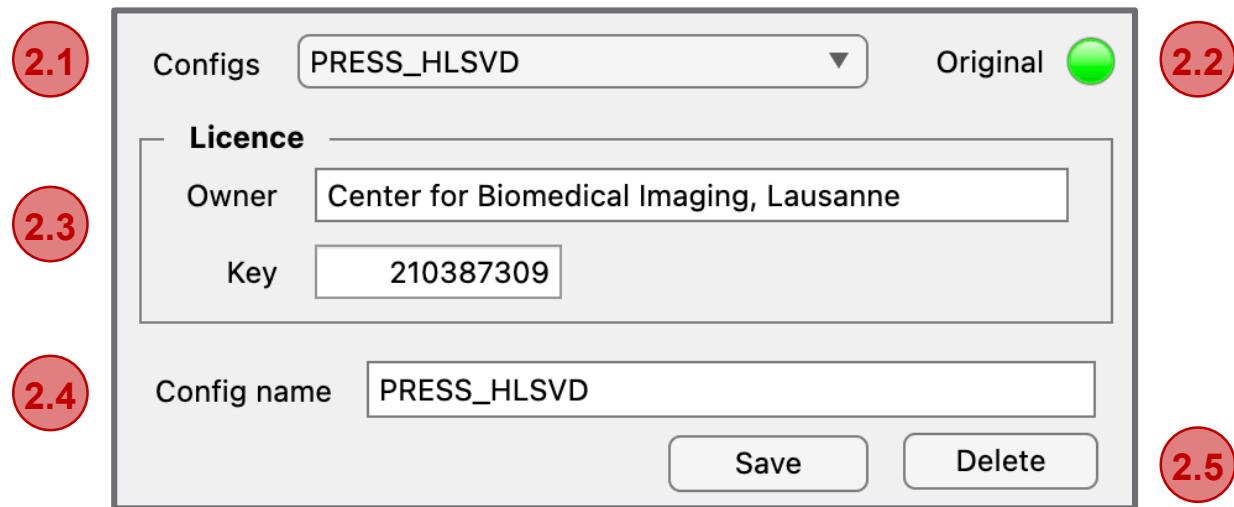
- LCModel path** and **Basis set** sections (highlighted by red circle 1):
 - Checkboxes for NSIMUL, VITRO, and NRATIO.
 - Input fields for PPM start (4), PPM end (0.2), DKNTMN (0.25).
 - Relative metabolite selection: Cr+PCr.
 - Relative concentration input field: 8.
- Configs** dropdown set to PRESS_HLSVD, **Original** button (highlighted by red circle 2) is green.
- Licence** section:
 - Owner: Center for Biomedical Imaging, Lausanne.
 - Key: 210387309.
- Config name** input field: PRESS_HLSVD.
- Save** and **Delete** buttons.
- Combination** section (highlighted by red circle 3):
 - NCOMB: 4.
 - Table: Index | Combination
 - 1 NAA+NAAG
 - 2 Glu+Gln
 - 3 GPC+PCho
 - 4 Cr+PCr
- Omission** section:
 - NOMIT: 15.
 - Table: Index | Omitted
 - 1 -CrCH2
 - 2 Gua
 - 3 Ser
 - 4 Lip13a
 - 5 Lip13b
 - 6 Lip09
 - 7 MM09
- Use** section:
 - NUSE: 7.
 - Table: Index | Used
 - 1 NAA
 - 2 Gln
 - 3 PCr
 - 4 Cr
 - 5 Ins
 - 6 Tau
 - 7 PCho
- Registration** section (highlighted by red circle 4):
 - Buttons: Template with skull, Template Brain mask, Anatomical segmentation, Segmentation labels.

1 - MRSI Parameters (Fitting, registration)

1.1	LCModel path	Basis set
1.3	<input type="checkbox"/> NSIMUL	PPM start <input type="text" value="4"/>
1.4	<input type="checkbox"/> VITRO	PPM end <input type="text" value="0.2"/>
1.5	<input checked="" type="checkbox"/> NRATIO	DKNTMN <input type="text" value="0.25"/>
	Relative metabolite	<input type="text" value="Cr+PCr"/>
	Relative concentration	<input type="text" value="8"/>

- 1.2 1.1. Path of LCModel software and executable
- 1.2 1.2. Basis set made by LCModel used for fitting and quantification
- 1.2 1.3. Simulated Lipids and MM (True or False)
- 1.6 1.4. INVITRO acquisition (True) INVIVO (False)
- 1.7 1.5. NRATIO : Soft constraints between metabolites (true : NRATIO = 12, false NRATIO = 0)
- 1.8 1.6. Start of ppm scale (reverse view)
- 1.8 1.7. End of ppm scale (reverse view)
- 1.9 1.8. DKNTMN value : space between each baseline point in ppm scale, control the stiffness of the baseline
- 1.9 1.9. Relative metabolite and its concentration

1 - MRSI Parameters (Fitting, registration)



2.1. Available configurations

2.2. Green if same as original saved configuration Red if some changes has been made

2.3. LCModel Licence : Owner & Key (As it is free, just keep the same key and modify the Owner with your lab)

2.4. Configuration name : To be changed to save a new configuration

2.5. Save or Delete the current configuration

1 - MRSI Parameters (Fitting, registration)

3.1 3.2 3.3

Combination	
NCOMB	4
Index	Combination
1	NAA+NAAG
2	Glu+Gln
3	GPC+PCho
4	Cr+PCr

Omission	
NOMIT	15
Index	Omitted
1	-CrCH2
2	Gua
3	Ser
4	Lip13a
5	Lip13b
6	Lip09
7	MM09

Use	
NUSE	7
Index	Used
1	NAA
2	Gln
3	PCr
4	Cr
5	Ins
6	Tau
7	PCho

3.1. Combination of metabolites from basis set

3.2. Omission of metabolites from basis set or simulated by LCModel

3.3. Metabolite names of the spectra to be used in the preliminary study

1 - MRSI Parameters (Fitting, registration)

Registration

Template with skull

Template Brain
mask

Anatomical
segmentation

Segmentation
labels

4.1

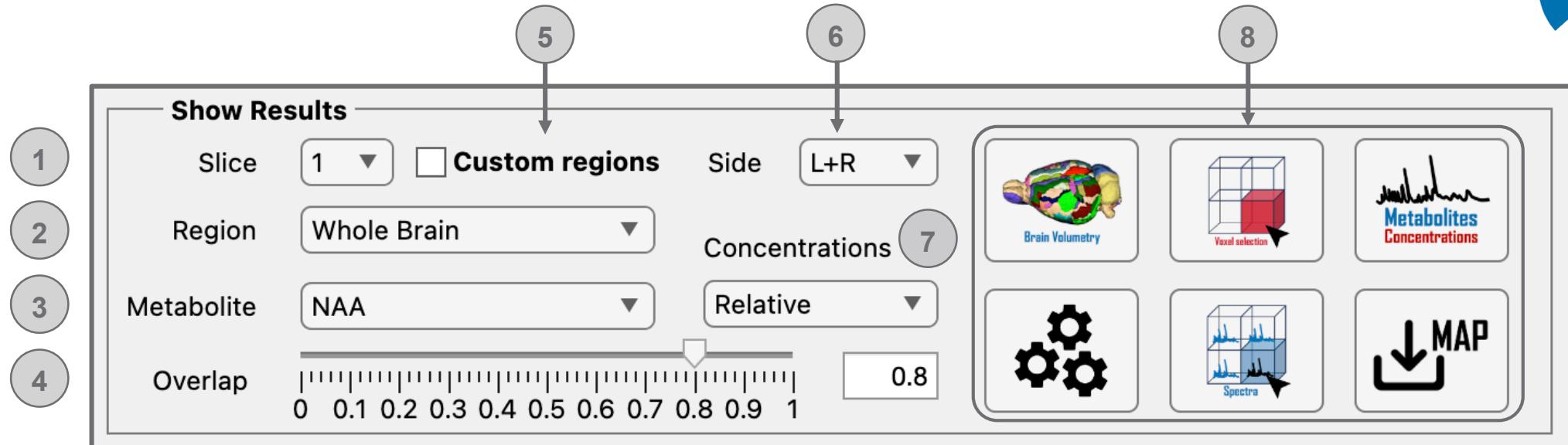
4.2

4.3

4.4

- 4.1. Anatomical template with skull and fat (.nii.gz files)
- 4.2. Anatomical template brain mask (removing skull and fat) (.nii.gz files)
- 4.3. Anatomical segmentation of the brain (labelling brain regions) (.nii.gz files)
- 4.4. Segmentation labels translation (.mat file)

1 - MRSI Results display



1. MRSI slice studied
2. Region list Dropdown
3. Metabolite list Dropdown
4. Minimum overlap between MRI voxels and MRSI voxels 0 - 1 voxel is sufficient, 1 - all MRI voxels must be in MRSI voxel
5. Combined regions from the region list with Left and Right possibilities
6. Side of the brain region : Left, Right and Left+Right
7. Concentrations : Absolute or Relative
8. Options (Brain volumetry, display options, manual voxel selection, spectra selection, Metabolites concentration, Save metabolite map)

1 - MRSI Results display



1.1

Volumetry table

Brain region	Left	Right	L+R
Olfactory bulb	52.82	54.01	106.83
Prelimbic cortex	20.92	20.4	41.32
Frontal Association Cortex	2.32	2.81	5.13
Cingulate cortex	25.78	22.74	48.52
Retrosplenial Cortex	29.5	27.54	57.04
Primary Motor Cortex	0	0	0
Secondary Motor Cortex	13.76	12.25	26.01
Primary Somatosensory Cortex	97.28	68.74	166.01
Secondary Somatosensory Cortex	7.67	7.99	15.67
Orbital Cortex	9.49	9.72	19.21
Insular Cortex	56.97	54.3	111.28
Amygdalopiriform Cortex	8.11	8.85	16.96
Entorhinal Cortex	49.49	59.08	108.57
Ectorhinal Cortex	12.35	12.71	25.06
Perirhinal Cortex	12.2	11.65	23.85
Primary Auditory Cortex	23.29	21.69	44.99
Secondary Auditory Cortex	11.77	10.46	22.23

1.2

Save name Save

- 1.1. Brain regions volumes Left, Right and L+R
- 1.2. Save volumetry into study folder

2.1

2.2

2.3

2.4

2.5

Display settings

MRS4BRAIN Toolbox

Quality controls

SNR Mean SNR 3.83
Minimum SNR ▾ 3

FWHM Mean FWHM 0.03709
Maximum threshold ▾ 1.25

Max CRLB limit [%] 100

Interpolation Off On

Automatic max concentration Max concentration 12

- 2.1. SNR quality control, minimal threshold of average or minimal value
- 2.2. Linewidth quality control, maximal threshold of average or maximal value
- 2.3. Maximal CRLB admitted after fitting (Cramer-Rao Lower Bound)
- 2.4. Interpolation of metabolite map (On/Off)
- 2.5. Automatic/Manual maximal concentration in metabolite map

1 - MRSI Results display



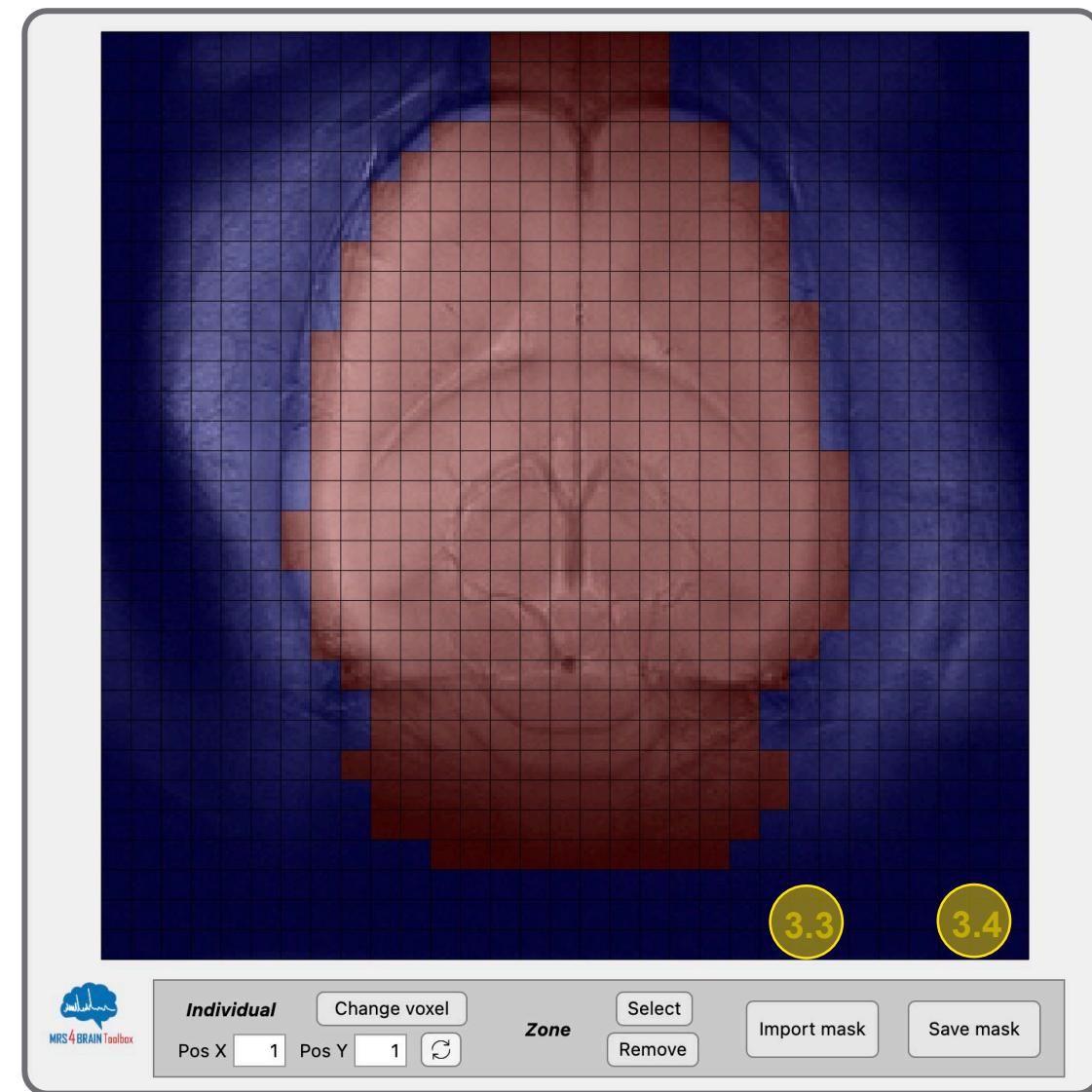
3.1. Change the voxel state between being activated and part of the applied mask or disactivated and removed from the applied mask

- Manual selection with cursor (Change voxel button)
- Give position X and Y and press the update button

3.2. Zoning : Select a zone that will be part of the brain mask or Remove a zone that do not belongs to the brain mask

3.3. Import a mask with same size as the MRSI matrix. Combine with the current mask or remove the current mask and replace it by the new one

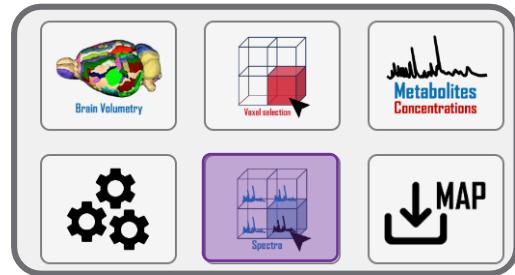
3.4. Save the mask in a "Mask" folder and change the display of the metabolite map in the MRSI main window



3.1

3.2

1 - MRSI Results display



4.1

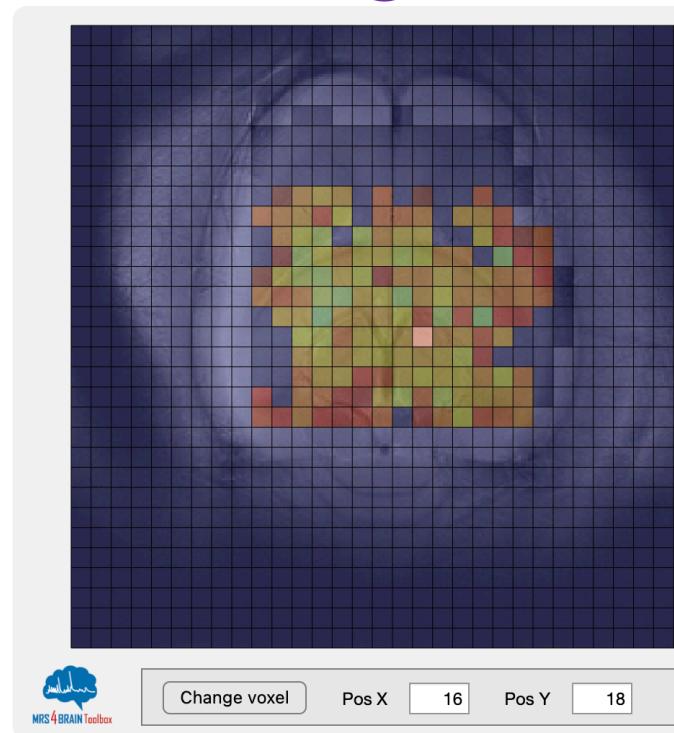
4.1. Spectrum selection window with anatomical image in background, metabolite map in middle ground, current voxel spectrum highlighted, and other available voxels fitted

4.2. Change voxel spectrum plotted by clicking on desired voxel, also update the position

4.3. Change spectrum plotted by giving the position

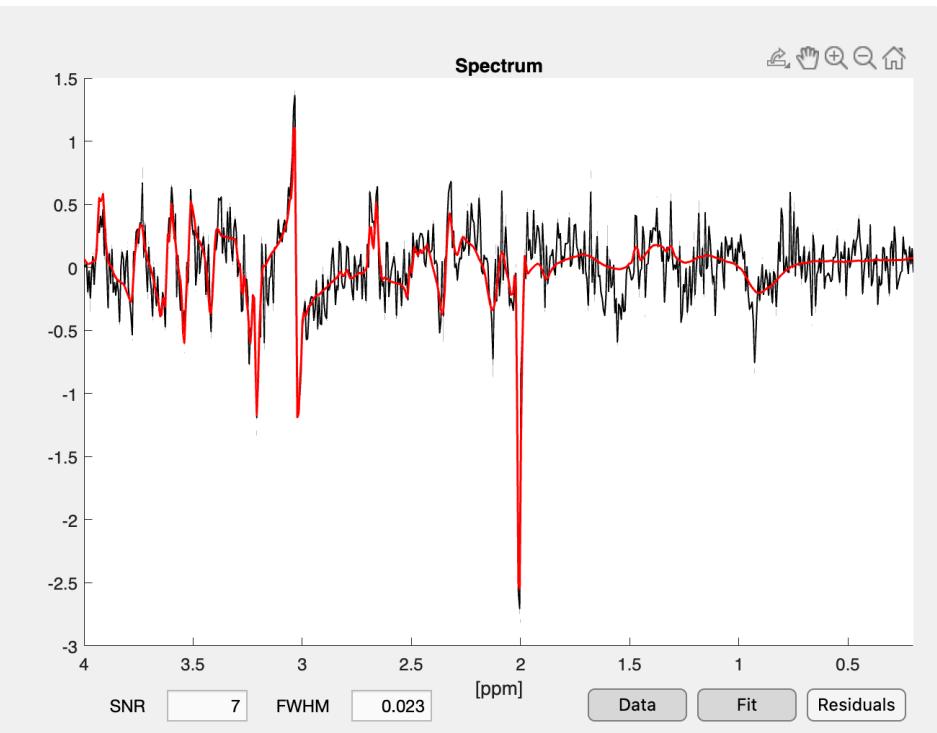
4.4. SNR and Linewidth calculated by LCModel on current spectrum

4.5. Display raw data, LCModel fit and residuals



4.2

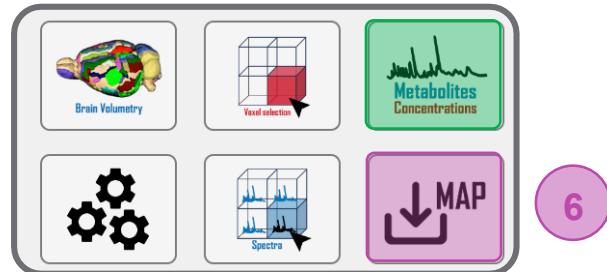
4.3



4.4

4.5

1 - MRSI Results display



6

5.1. Table of metabolite concentrations on current mask and with the quality controls applied

- Metabolite name
- Mean concentration over the metabolite map voxels
- Standard deviation of the concentration over the metabolite map voxels
- Number of voxels that are used for statistics from quality controls

5.2. Save the metabolite concentration table to be used for statistics

6. Save current metabolite map displayed in the MRS4Brain main window / MRSI as .png and .fig files

Concentration table 5.1

Metabolite	Mean	Std	N voxels
Mac	0.00	0.00	143
Cr	4.43	1.51	140
PCr	4.05	1.24	130
Ins	9.51	1.60	144
NAA	10.88	1.63	144
Tau	7.52	1.56	144
PCho	1.38	0.58	124
GPC	0.94	0.43	72
Glu	8.80	1.76	144
Gln	2.80	0.92	142
Ala	1.29	0.44	17
Asc	3.65	1.38	98
Asp	1.57	0.47	105
GABA	1.19	0.39	135
Glc	1.05	0.27	135
GSH	1.20	0.43	136
Lac	1.78	1.01	21

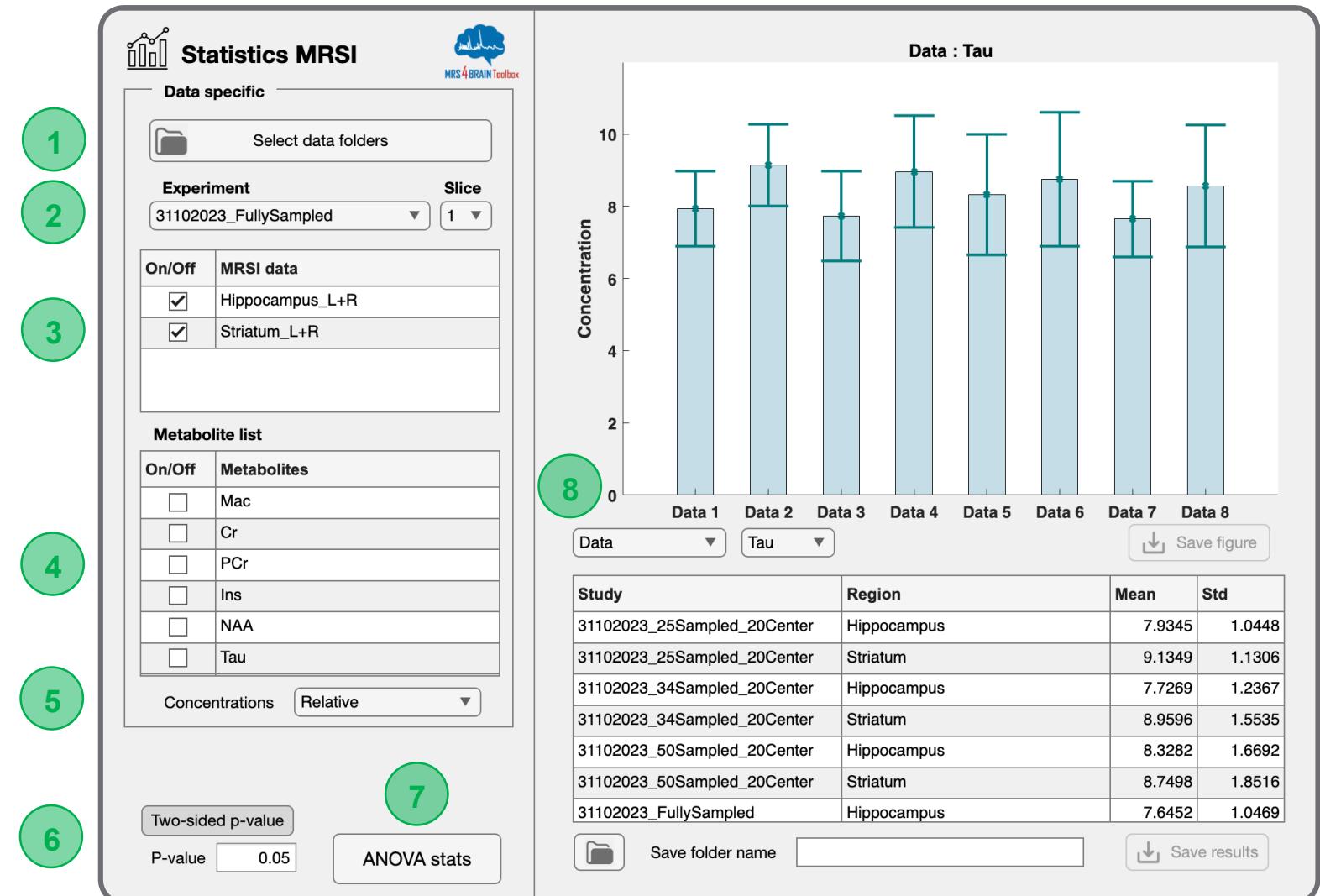
Save name

Save

5.2

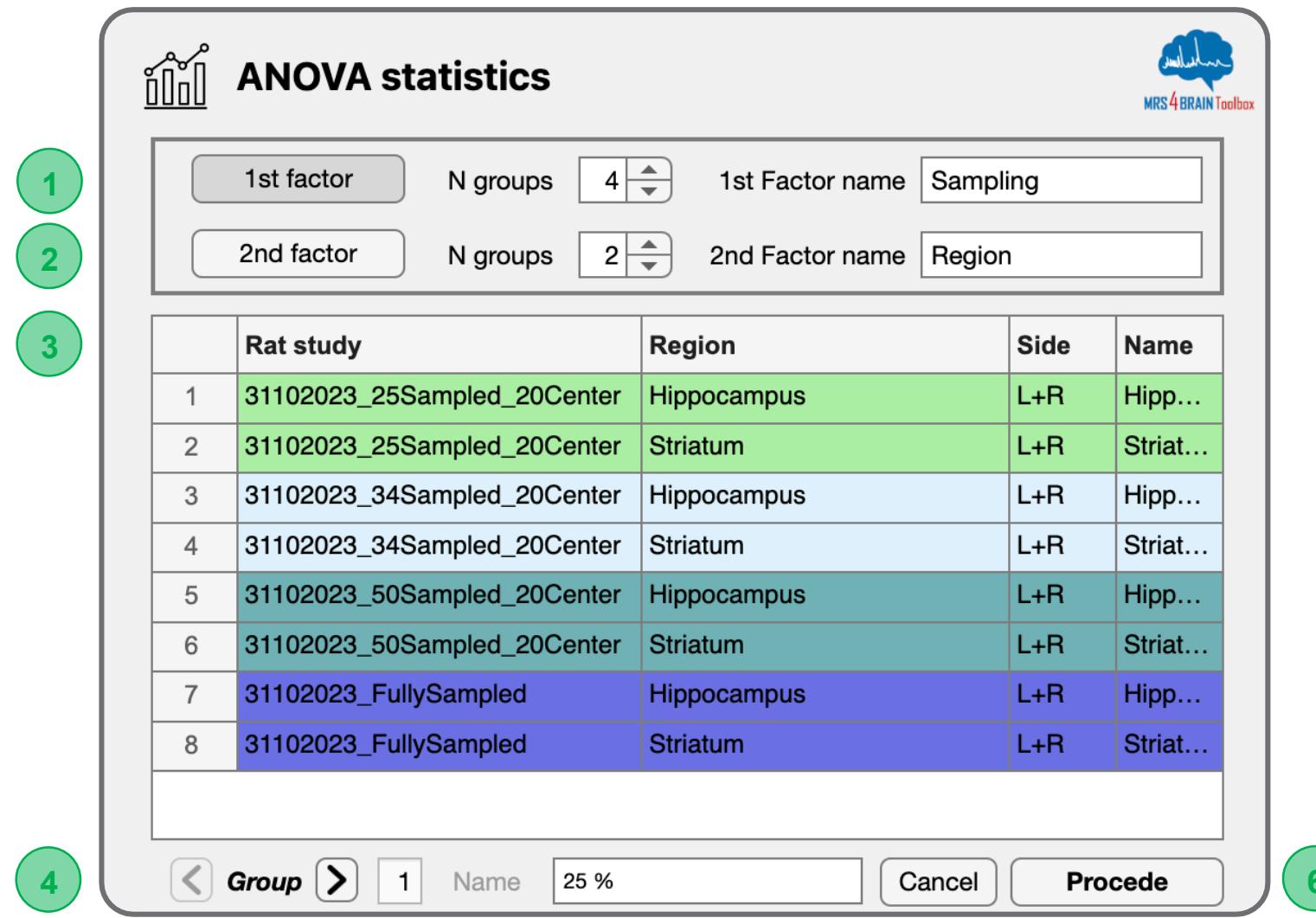
1 - MRSI Statistics

1. Select folder with MRSI study folders
2. Choose experiment/study dropdown and slice
3. Saved MRSI data (metabolites, mean, std, number of voxels) and select the ones for statistics
4. Metabolite list available for statistics
5. Relative or Absolute concentration
6. P-value for significant difference, one or two tailed T-test
7. ANOVA statistics window opening or T-test calculation
8. Plot of statistics data for the selected metabolite on the dropdown + region, mean and std in the table



1 - MRSI Statistics

1. 1st ANOVA factor selection, with number of groups and name of this factor
2. 2nd ANOVA factor selection, with number of groups and name of this factor
3. Table of rat studies and by clicking on the group wanted, change the color and make the groups as wanted
4. Navigation between the different groups to modify the table
5. Change name of the current group
6. Proceed ANOVA 1 or 2 ways with the groups made



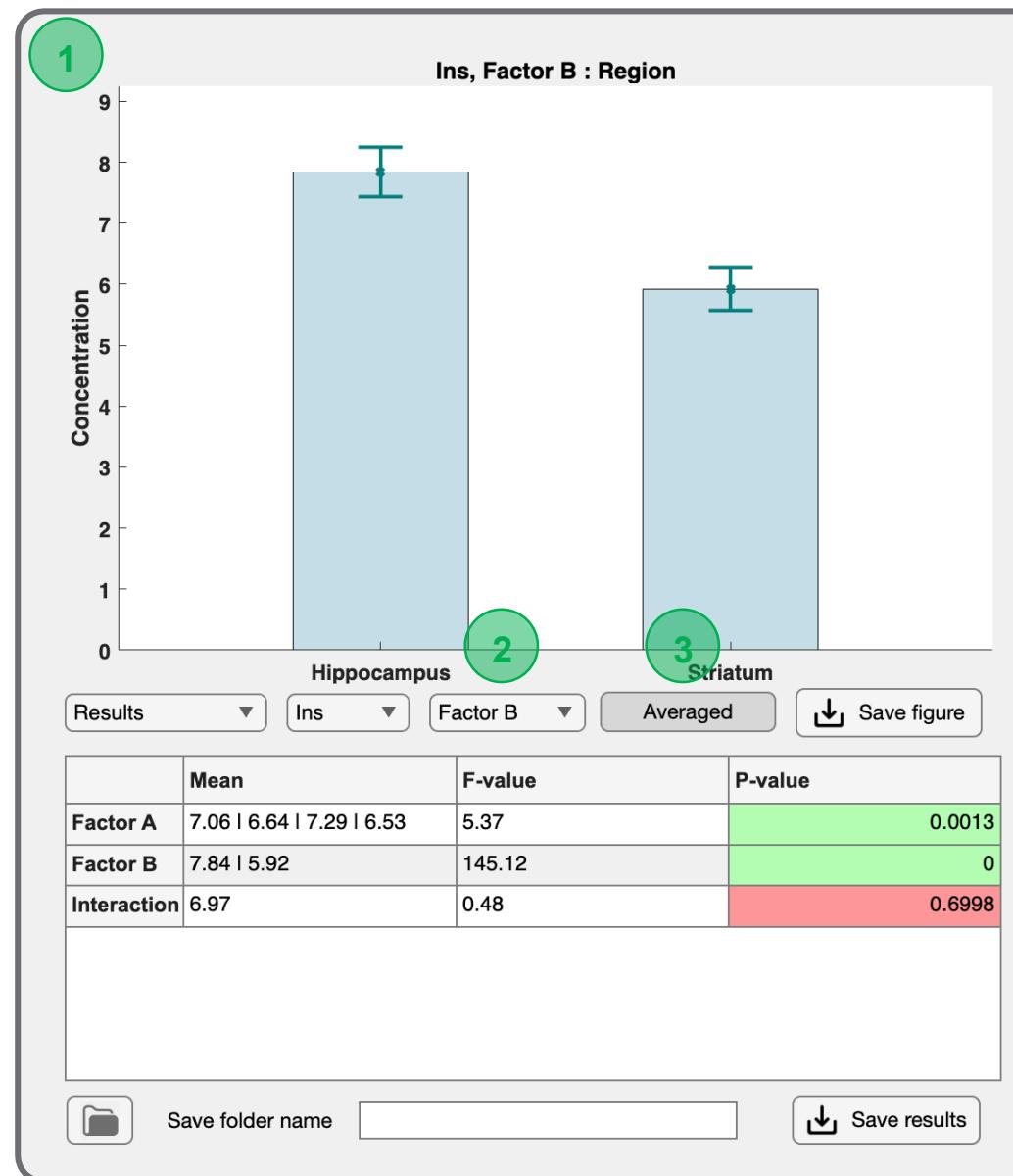
ANOVA statistics

	Rat study	Region	Side	Name
1	31102023_25Sampled_20Center	Hippocampus	L+R	Hipp...
2	31102023_25Sampled_20Center	Striatum	L+R	Striat...
3	31102023_34Sampled_20Center	Hippocampus	L+R	Hipp...
4	31102023_34Sampled_20Center	Striatum	L+R	Striat...
5	31102023_50Sampled_20Center	Hippocampus	L+R	Hipp...
6	31102023_50Sampled_20Center	Striatum	L+R	Striat...
7	31102023_FullySampled	Hippocampus	L+R	Hipp...
8	31102023_FullySampled	Striatum	L+R	Striat...

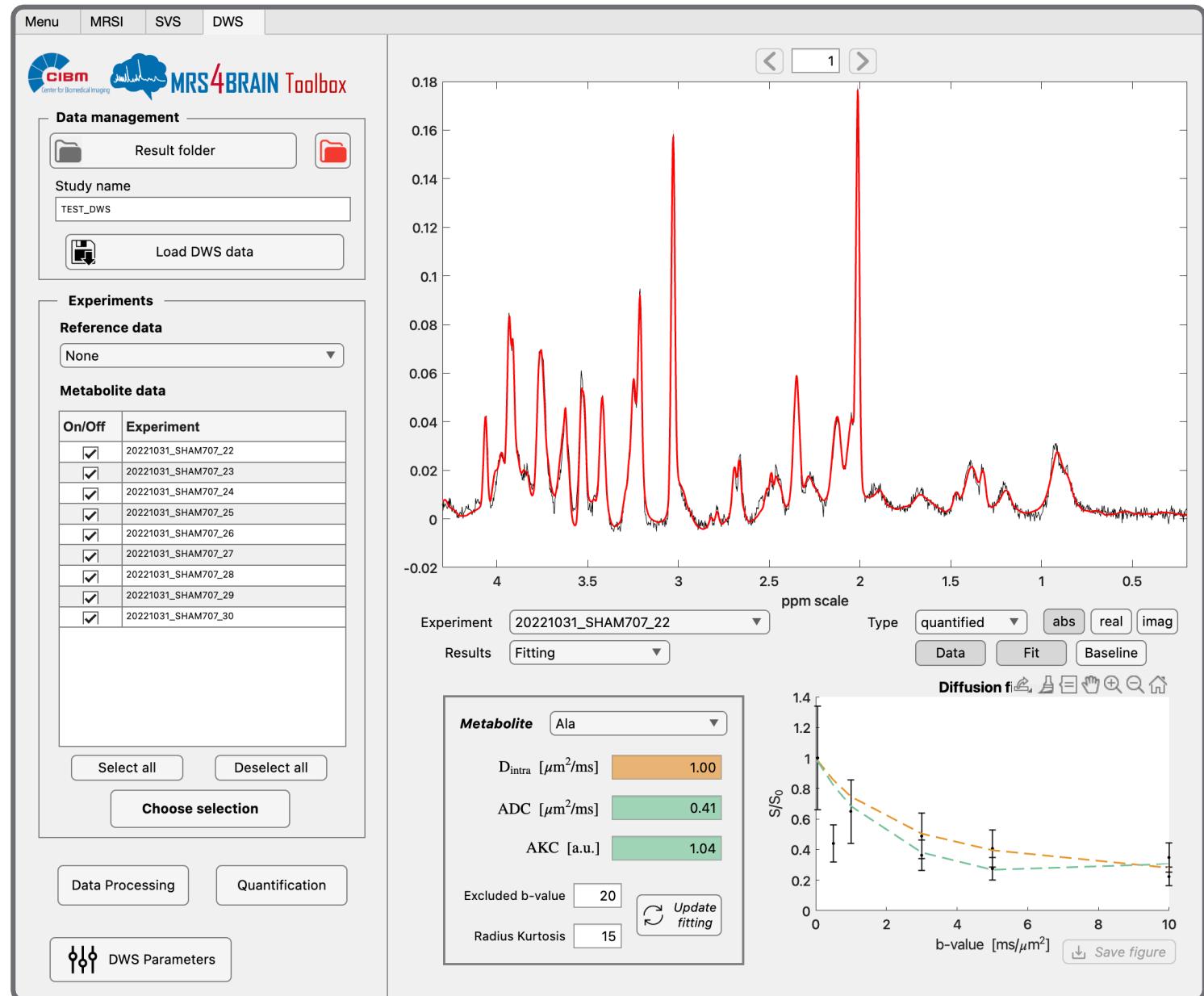
1 2 3 4 5 6

1 - MRSI Statistics

1. Plot of statistics for T-test, ANOVA 1 or 2 ways
2. Choose between Factor A or B of ANOVA
3. Single or Averaged study results
4. Results table with mean values, F-value and P-value with green for significant and red for insignificant
5. Save T-test, ANOVA results in a folder as well as figures



3 - DWS



3 - DWS

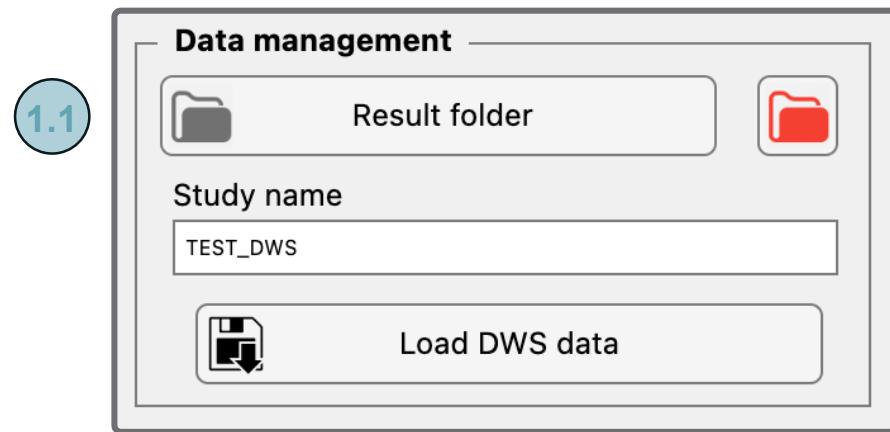
Bruker data management

Preprocessing steps

Parameters
(Fitting, preprocessing)



3 - DWS BRUKER Data Management

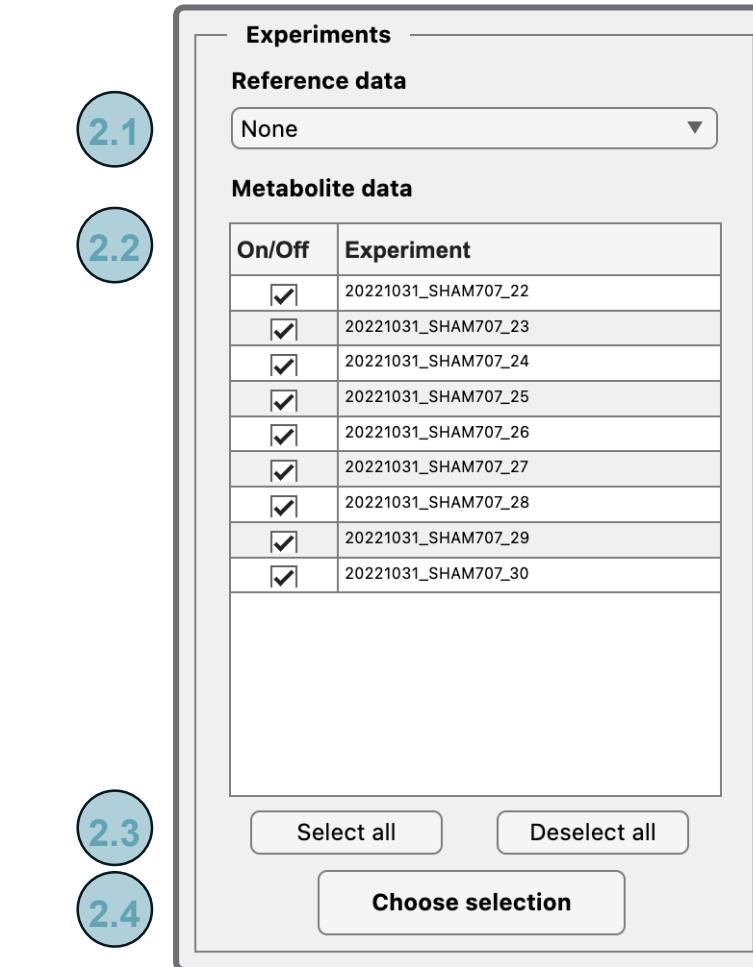


1.1. Selection of a result folder (where the study will be saved)

1.2. Selection of a study folder

1.3. Name of the study - where the results will be saved

1.4. Load dMRS data into another window



On/Off	Experiment
<input checked="" type="checkbox"/>	20221031_SHAM707_22
<input checked="" type="checkbox"/>	20221031_SHAM707_23
<input checked="" type="checkbox"/>	20221031_SHAM707_24
<input checked="" type="checkbox"/>	20221031_SHAM707_25
<input checked="" type="checkbox"/>	20221031_SHAM707_26
<input checked="" type="checkbox"/>	20221031_SHAM707_27
<input checked="" type="checkbox"/>	20221031_SHAM707_28
<input checked="" type="checkbox"/>	20221031_SHAM707_29
<input checked="" type="checkbox"/>	20221031_SHAM707_30

Select all Deselect all

Choose selection

2.1. Choose a reference signal (if there is one) for the study

2.2. Choose metabolite experiment data

2.3. Select all or Deselect all the metabolite experiment data in the table

2.4. Validate the selection of reference and metabolite data and start the DWS processing by reading the files and creating raw study files (saved in the study folder)

3 - DWS BRUKER Data Management

1.1

1.2

1.3

1.4

1.5

1.6

On/Off	Nº exp	saved name
<input type="checkbox"/>	7	20221031_SHAM707_week4_7
<input type="checkbox"/>	8	20221031_SHAM707_week4_8
<input type="checkbox"/>	10	20221031_SHAM707_week4_10
<input type="checkbox"/>	13	20221031_SHAM707_week4_13
<input type="checkbox"/>	15	20221031_SHAM707_week4_15
<input type="checkbox"/>	16	20221031_SHAM707_week4_16
<input type="checkbox"/>	17	20221031_SHAM707_week4_17
<input type="checkbox"/>	19	20221031_SHAM707_week4_19
<input type="checkbox"/>	20	20221031_SHAM707_week4_20
<input checked="" type="checkbox"/>	22	20221031_SHAM707_week4_22
<input checked="" type="checkbox"/>	23	20221031_SHAM707_week4_23
<input checked="" type="checkbox"/>	24	20221031_SHAM707_week4_24
<input checked="" type="checkbox"/>	25	20221031_SHAM707_week4_25
<input checked="" type="checkbox"/>	26	20221031_SHAM707_week4_26

- 1.1. Open a Bruker data folder and fill the table with the experiment inside
- 1.2. PDF document : Open the Bruker data folder and allow user to open a PDF document to look at an experiment sheet with exp numbers
- 1.3. Update the base name of the study to avoid long names and be more specific
- 1.4. Experiment table : Select the experiment wanted, the folder number and can also edit the saved name
- 1.5. Select all or deselect all the experiments in the table
- 1.6. Load the experiment data into the MRS4Brain main window and fill the reference data dropdown and metabolite data table

3 - DWS Parameters (Fitting, Preprocessing)

1

2

Preferences SVS/DWS

LCModel path	Basis set	Configs DWS_14T_1H_isison	Original																																									
<input type="checkbox"/> NSIMUL	PPM start 4.3	Licence																																										
<input type="checkbox"/> VITRO	PPM end 0.2	Owner Center for Biomedical Imaging, Lausanne																																										
<input checked="" type="checkbox"/> NRATIO	DKNTMN 0.25	Key 210387309																																										
Relative metabolite Cr+PCr	Config name DWS_14T_1H_isison	Save	Delete																																									
Relative concentration 8																																												
Combination NCOMB 4	Omission NOMIT 15	Use NUSE 7																																										
<table border="1"><thead><tr><th>Index</th><th>Combination</th></tr></thead><tbody><tr><td>1</td><td>NAA+NAAG</td></tr><tr><td>2</td><td>Glu+Gln</td></tr><tr><td>3</td><td>GPC+PCho</td></tr><tr><td>4</td><td>Cr+PCr</td></tr></tbody></table>	Index	Combination	1	NAA+NAAG	2	Glu+Gln	3	GPC+PCho	4	Cr+PCr	<table border="1"><thead><tr><th>Index</th><th>Omitted</th></tr></thead><tbody><tr><td>1</td><td>-CrCH2</td></tr><tr><td>2</td><td>Gua</td></tr><tr><td>3</td><td>Ser</td></tr><tr><td>4</td><td>Lip13a</td></tr><tr><td>5</td><td>Lip13b</td></tr><tr><td>6</td><td>Lip09</td></tr><tr><td>7</td><td>MM09</td></tr></tbody></table>	Index	Omitted	1	-CrCH2	2	Gua	3	Ser	4	Lip13a	5	Lip13b	6	Lip09	7	MM09	<table border="1"><thead><tr><th>Index</th><th>Used</th></tr></thead><tbody><tr><td>1</td><td>NAA</td></tr><tr><td>2</td><td>Gln</td></tr><tr><td>3</td><td>PCr</td></tr><tr><td>4</td><td>Cr</td></tr><tr><td>5</td><td>Ins</td></tr><tr><td>6</td><td>Tau</td></tr><tr><td>7</td><td>PCho</td></tr></tbody></table>	Index	Used	1	NAA	2	Gln	3	PCr	4	Cr	5	Ins	6	Tau	7	PCho
Index	Combination																																											
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6	Tau																																											
7	PCho																																											
Pre processing																																												
Fid-A steps : <input checked="" type="checkbox"/> Align averages <input checked="" type="checkbox"/> Outliers removal																																												
Line Broadening 12	Rejection threshold 1.5	ISIS																																										
Frequency range [ppm] : min 7	max 8	Maximum time 0.5																																										

1. Same as for MRSI
2. Preprocessing steps and parameters

3 - DWS Parameters (Fitting, Preprocessing)

Pre processing

Fid-A steps : Align averages Outliers removal

Line Broadening Rejection threshold

Frequency range [ppm] : min max Maximum time

2.2

ISIS

2.1

2.3

2.1. Select Fid-A steps

2.2. Image-Selected In vivo Spectroscopy (ISIS) On : e.g. SPECIAL, OFF : e.g. STEAM

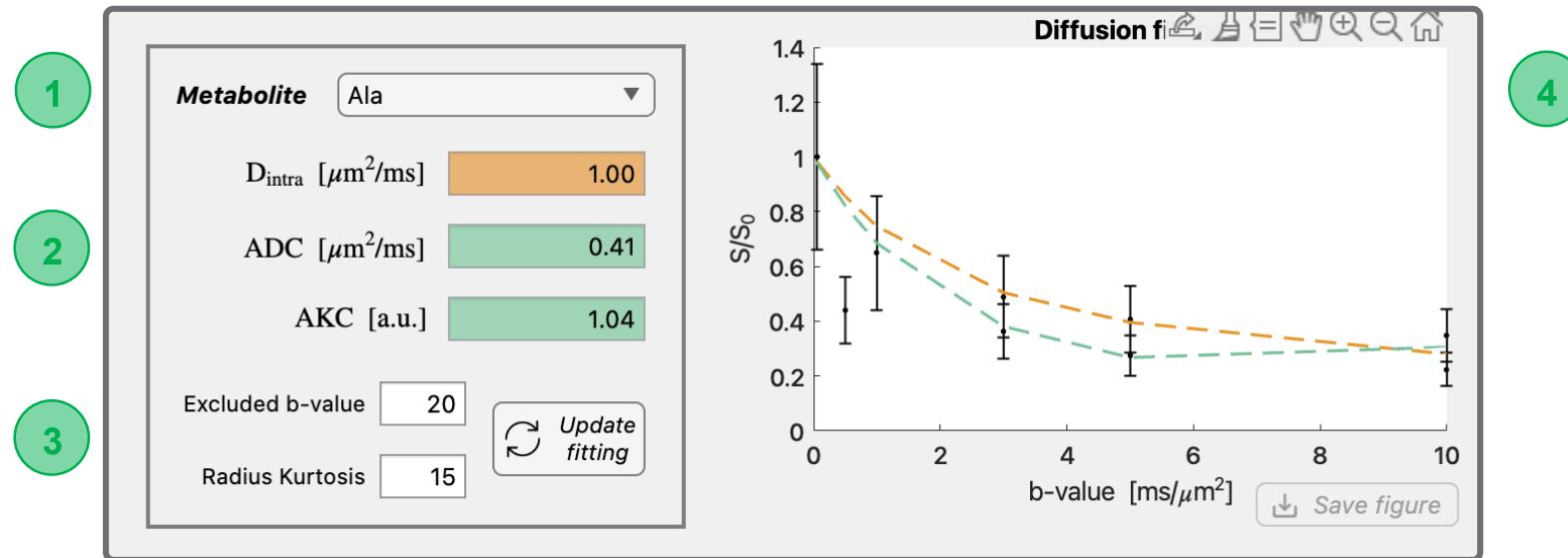
2.3. Fid-A preprocessing parameters : SEE WITH JM

3 - DWS Processing Steps

1. **Choose selection button** : Validate the selection of reference and metabolite data and start the DWS processing by reading the files and creating raw study files (saved in the study folder)
2. **Data processing button** : Preprocess the data with Fid-A functions (Align Averages (shots) and Remove outliers) and then the individual shots are summed, and new process study files are created and saved in the study folder
3. **Quantification button** : LCModel fitting of spectra with or without reference, quantification and extraction of metabolites data, fits and biological modelling. Create LCModel files available in quantified folder in the study folder

Nom	Date de modification	Taille	Type
20221031_AM_DWS_experiment.mat	14 novembre 2023 à 12:38	170.2 Mo	MATLAB Data
> Figures	avant-hier à 14:10	--	Dossier
> processed	14 novembre 2023 à 11:50	--	Dossier
> quantified	14 novembre 2023 à 12:02	--	Dossier
> raw	14 novembre 2023 à 11:49	--	Dossier

3 - DWS



1. Select fitted metabolite
2. Diffusion coefficient for 2 different modelling :
 - oriented sticks (1) : $\frac{S}{S_0} = \sqrt{\frac{\pi}{4b * D_a}} * \text{erf}(\sqrt{b * D_a})$ with $b = \text{b-value}$, $D_a = D_{\text{intra}}$, erf (error function)
 - Kurtosis (2,3) : $\frac{S}{S_0} = \exp\left(-b * D + \frac{1}{6} * b^2 * D^2 * K\right)$ with $b = \text{b-value}$, $D = \text{ADC}$, $K = \text{AKC}$.

3. Excluded b-value above the value selected and radius of convergence for Kurtosis modelling, can be updated anytime
4. Diffusion coefficient plot with orange = Oriented sticks model, green = Kurtosis model

3 - DWS - Spectra Display

1. Experiment Dropdown selection
2. Results (Concentrations table or fitting)
3. Type of steps/process : raw (raw data), processed (preprocessing applied on data without summing), processed + sum (same as processed but with summing) and quantified (LCModel fitting with processed + sum data)
4. abs (absolute value of data), real (real part of data), imag (imaginary part of data)
5. Quantified data option : see data, fit and baseline individually
6. Navigate through the different shots

