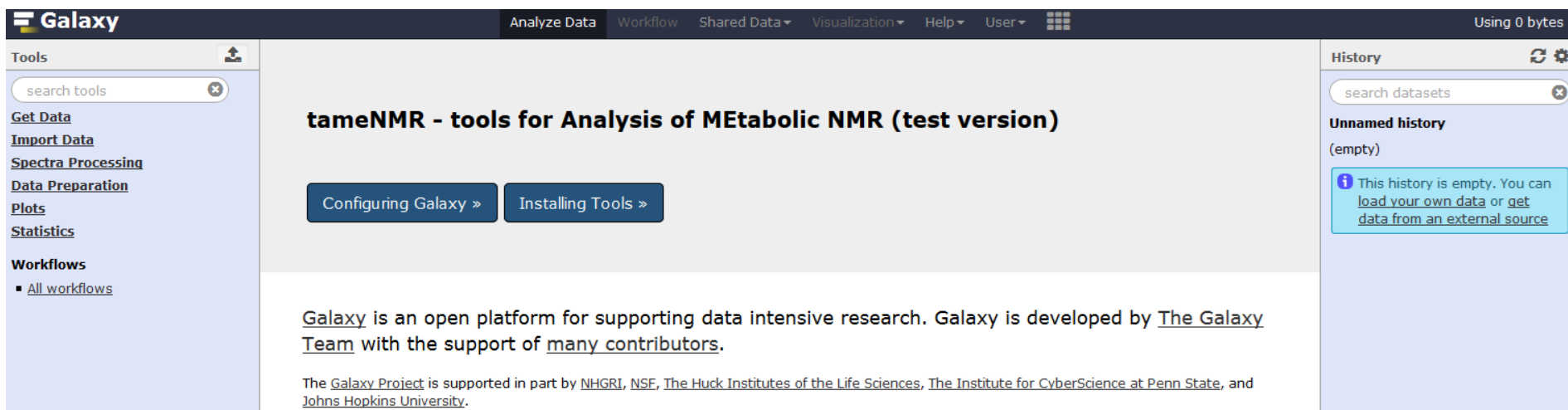


# NMR Metabolomics Workshop

## Appraisal of 1D spectra using tameNMR



The screenshot shows the Galaxy web interface. The top navigation bar includes 'Galaxy', 'Analyze Data', 'Workflow', 'Shared Data', 'Visualization', 'Help', and 'User'. The left sidebar contains a 'Tools' section with a search bar and links for 'Get Data', 'Import Data', 'Spectra Processing', 'Data Preparation', 'Plots', 'Statistics', and 'Workflows'. The main content area displays the 'tameNMR - tools for Analysis of METabolic NMR (test version)' tool page, which includes buttons for 'Configuring Galaxy' and 'Installing Tools'. Below these buttons, a paragraph describes Galaxy as an open platform for data-intensive research, developed by The Galaxy Team. The right sidebar shows a 'History' section with a search bar and a message indicating that the history is empty.

**Galaxy** | Analyze Data | Workflow | Shared Data | Visualization | Help | User | Using 0 bytes

**Tools** | search tools

[Get Data](#)  
[Import Data](#)  
[Spectra Processing](#)  
[Data Preparation](#)  
[Plots](#)  
[Statistics](#)  
**Workflows**  
▪ [All workflows](#)

### tameNMR - tools for Analysis of METabolic NMR (test version)

[Configuring Galaxy »](#) [Installing Tools »](#)

Galaxy is an open platform for supporting data intensive research. Galaxy is developed by [The Galaxy Team](#) with the support of [many contributors](#).

The [Galaxy Project](#) is supported in part by [NHGRI](#), [NSF](#), [The Huck Institutes of the Life Sciences](#), [The Institute for CyberScience at Penn State](#), and [Johns Hopkins University](#).

**History** | search datasets

**Unnamed history**  
(empty)

**i** This history is empty. You can [load your own data](#) or [get data from an external source](#)



23<sup>rd</sup> June 2019



# Workshop Structure

Open-Access Datasets  
(*what to deposit and how to access NMR data*)



1D NMR Analysis  
(*Raw Spectra visualisation,  
Annotation  
& Statistical analysis*)

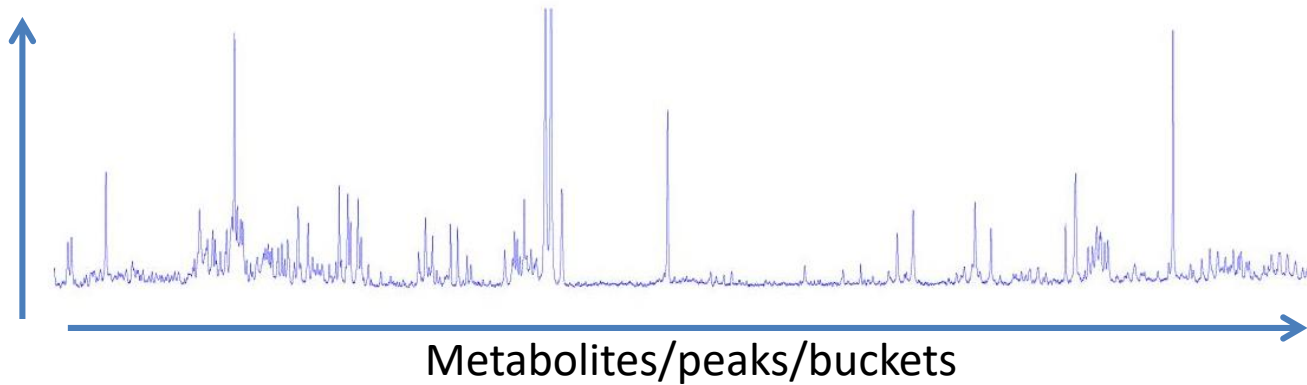


2D NMR analysis  
(*Metabolite Verification/Identification*)



**Section 2.** Accessing data downloaded from MetaboLights via Galaxyproject.org tool tameNMR (available via PhenoMeNal) and other tools available via workflow4metabolomics. This section will look at raw 1D <sup>1</sup>H NMR spectra deposited and bin spectra according to annotation provided with deposition and perform simple statistics on the resultant spectra intensity files..

# Spectral Formatting



Transformation of a  
Spectrum  
*Only useful to NMR  
spectroscopists using  
specific software*

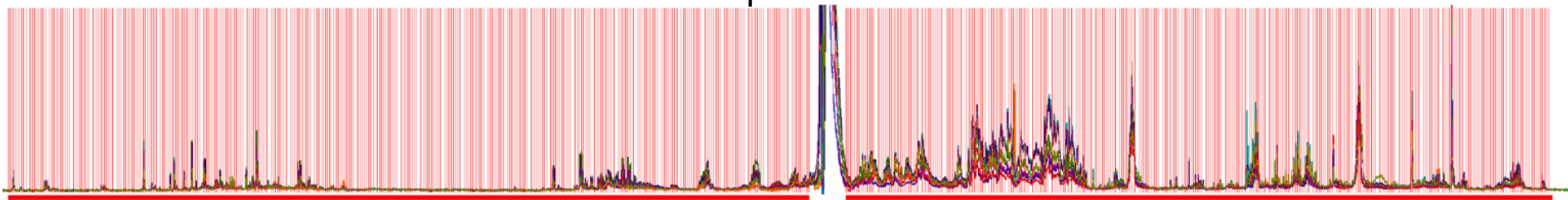
samples

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1		Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6	Pseudo_6
2	9.99975	3.86E-05	8.23E-06	1.36E-05	3.38E-05	2E-07	2.6E-05	-5.7E-05	-3.6E-05	2.35E-05	4.48E-05	-3E-06	-4.4E-06	-5.6E-06	0.000026
3	9.99925	3.49E-05	-5.1E-07	1.4E-05	1.67E-05	1.43E-05	8.16E-06	-6.5E-05	2.02E-05	0.000026	2.89E-05	-2.1E-05	6.82E-05	-2E-06	2.15E-05
4	9.99875	-6.5E-06	6.67E-06	3.38E-05	2.69E-05	1					.48E-05	-2.1E-05	4.57E-05	2.76E-06	3.77E-05
5	9.99825	-9E-06	-5.5E-06	5.06E-05	1.35E-05	-	intensity values				.83E-05	7.01E-06	1.96E-05	1.47E-05	4.65E-05
6	9.99775	-2.1E-05	-1.2E-05	5.25E-05	-3.6E-05	-					.22E-06	2.21E-05	4.1E-05	1.11E-05	4.06E-05
7	9.99725	-1.7E-05	-1.1E-05	5.91E-05	-5E-05	-2.6E-05	1.06E-05	3.35E-05	4.13E-05	3.09E-06	7.63E-06	2.58E-05	3.46E-05	2.37E-05	2.01E-05
8	9.99675	-2.5E-06	-2.1E-05	9.55E-06	-1.9E-05	-2.4E-06	1.4E-05	8.02E-06	-3.9E-07	-2.1E-05	5.63E-06	9.77E-06	2.61E-05	4.96E-05	2.65E-06
9	9.99625	5.85E-06	-1.2E-05	-2.5E-05	6.78E-06	-4.6E-06	-1.1E-06	2.29E-05	-1.5E-05	1.68E-05	1.01E-05	1.42E-05	2.21E-05	4.51E-05	1.67E-05
10	9.99575	-4.6E-07	-2.5E-05	-6.9E-06	-9E-06	-1.7E-05	1.49E-05	7.39E-05	-3.3E-05	3.42E-05	0.000017	-5.4E-06	2.76E-05	2.59E-05	6.22E-06
11	9.99525	-3E-06	-8.2E-06	-1.2E-05	-1.8E-05	-2.2E-05	1.72E-05	7.91E-05	-2.7E-05	3.5E-05	3.24E-05	-1E-05	1.79E-05	1.15E-05	7.5E-06
12	9.99475	-3.8E-06	3.99E-05	4.84E-05	-5.5E-05	-3.7E-06	2.85E-05	3.54E-05	-1.6E-06	1.9E-05	4.84E-05	-1.9E-05	6.39E-05	2.51E-05	1.82E-06

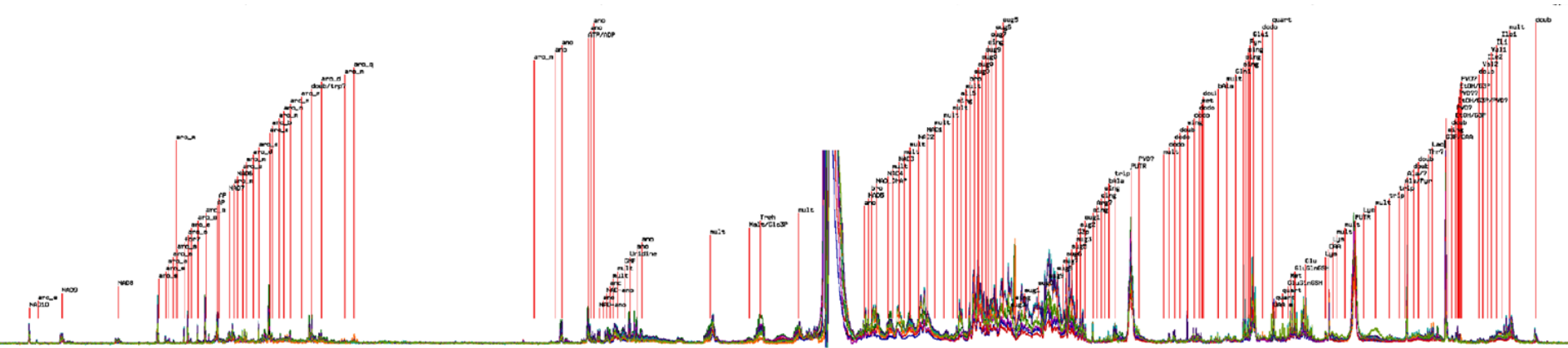
Into a Matrix of  
numbers.  
*Interpretation by  
multiple analysts and  
tools*

# Preparing a Bucket Table/Binning Spectra

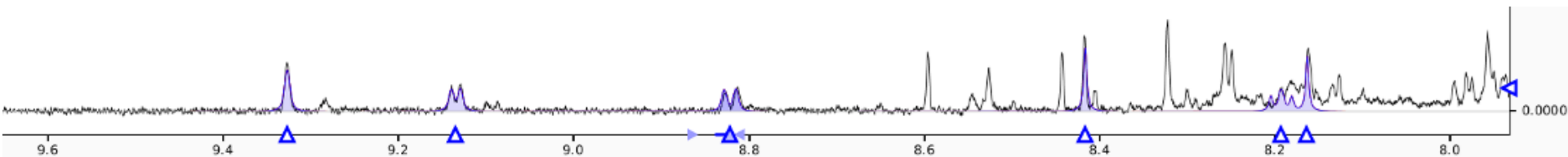
Options



1. divide spectrum into equal increments and integrate intensity for each increment



2. divide spectrum up into individual peaks and integrate intensity of each peak/group of peaks (requires a **pattern** file)



3. peak deconvolution via fitting wave functions (batman, Chenomx etc.)

# Incremental Bucketing

## Advantages:

- .Quick
- .Consistent
- .Unbiased
- .Useful for a first check

## Limitations:

- .No metabolite information
- .Could include artefact/contaminant peaks
- .Larger number of buckets

# Bucketing *via* Pattern File

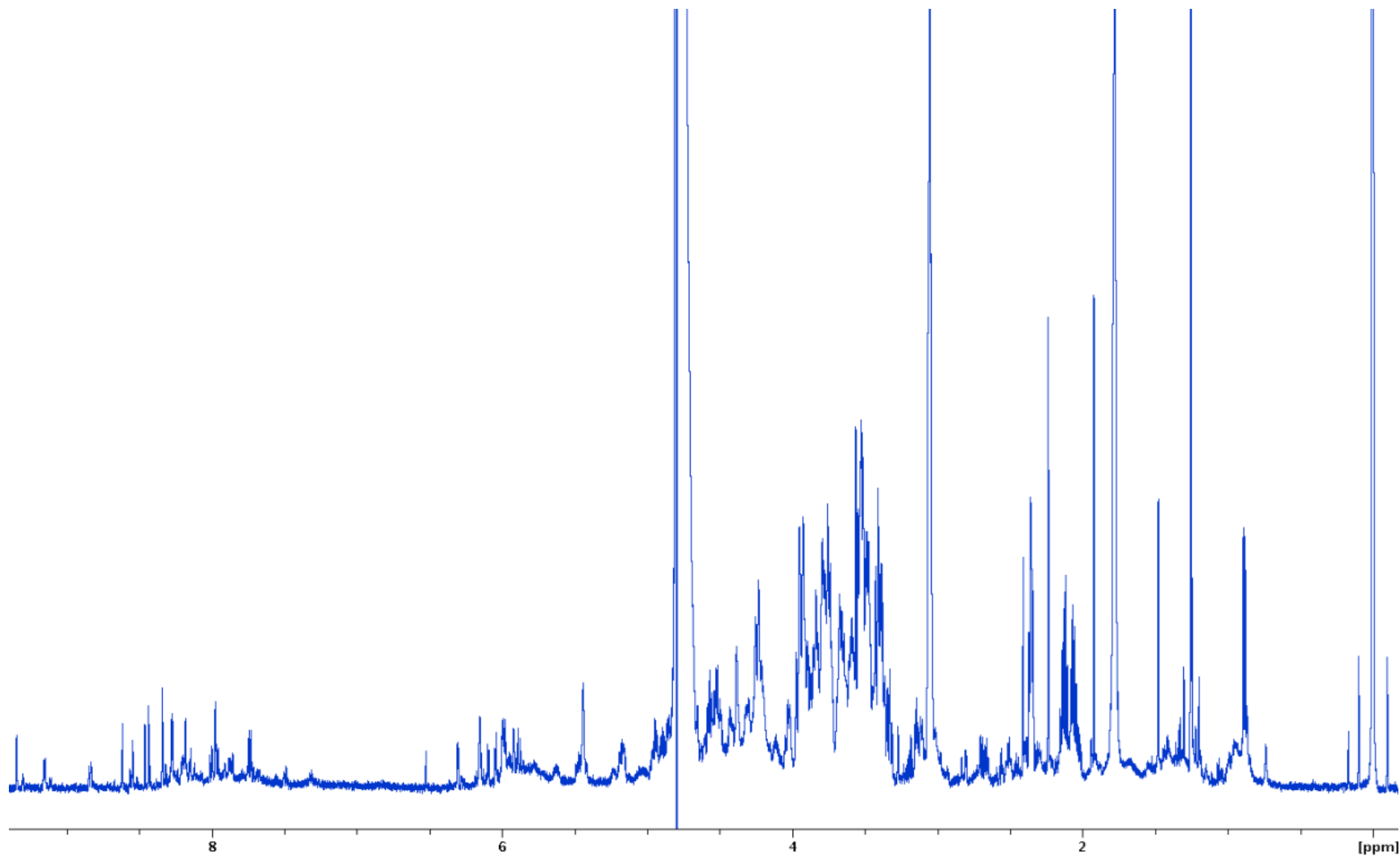
## Advantages:

- .All peaks represented
- .Removal of noise
- .Analysis can be metabolite driven
- .Intensities reflect the individual molecules

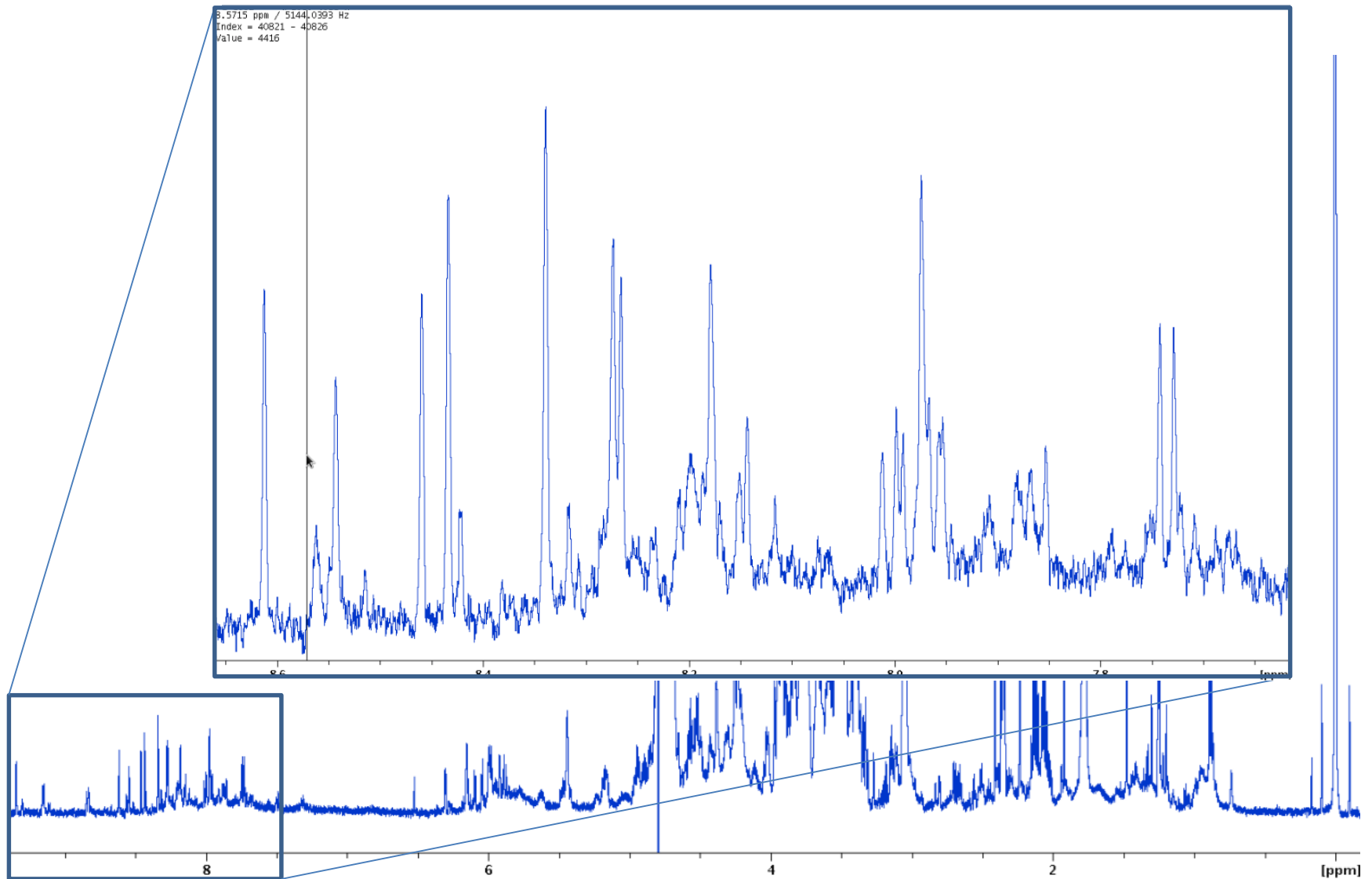
## Limitations:

- .Time consuming
- .Fiddly (need to be precise)
- .Need to assign metabolite to peaks to get the maximum benefit.

# Preparing a Pattern File

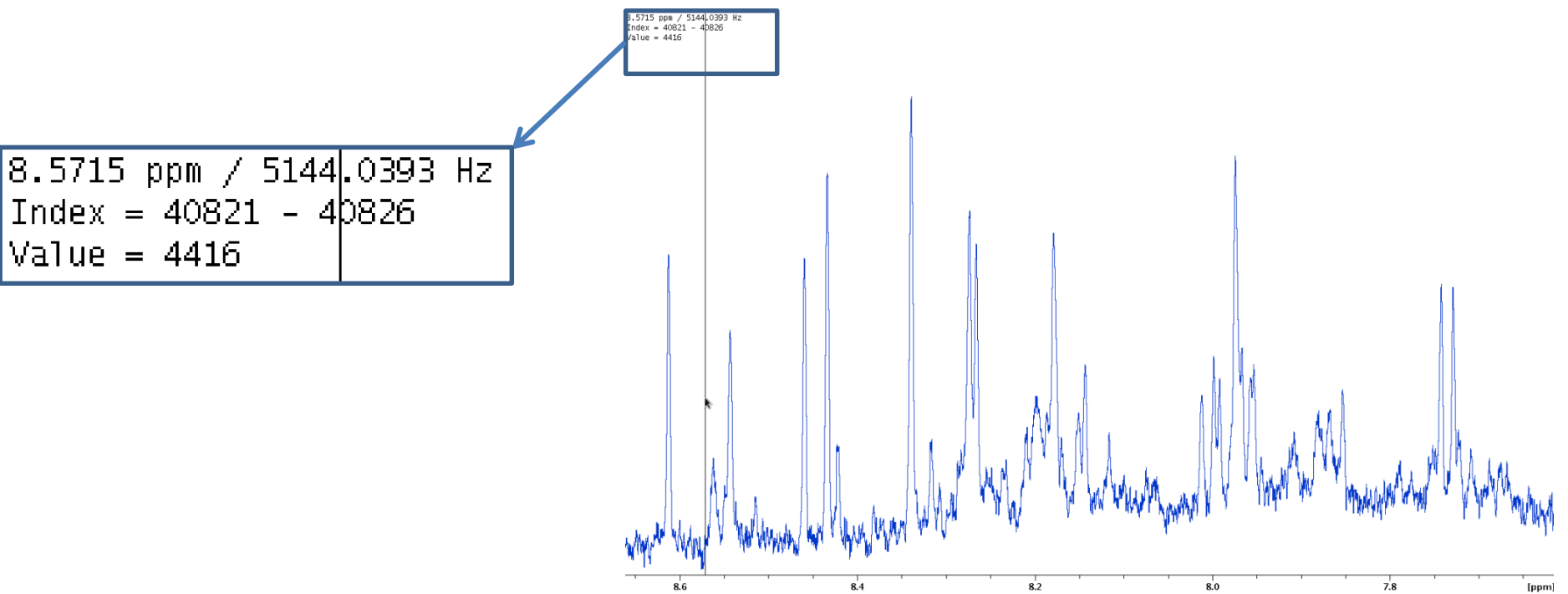


# Preparing a Pattern File

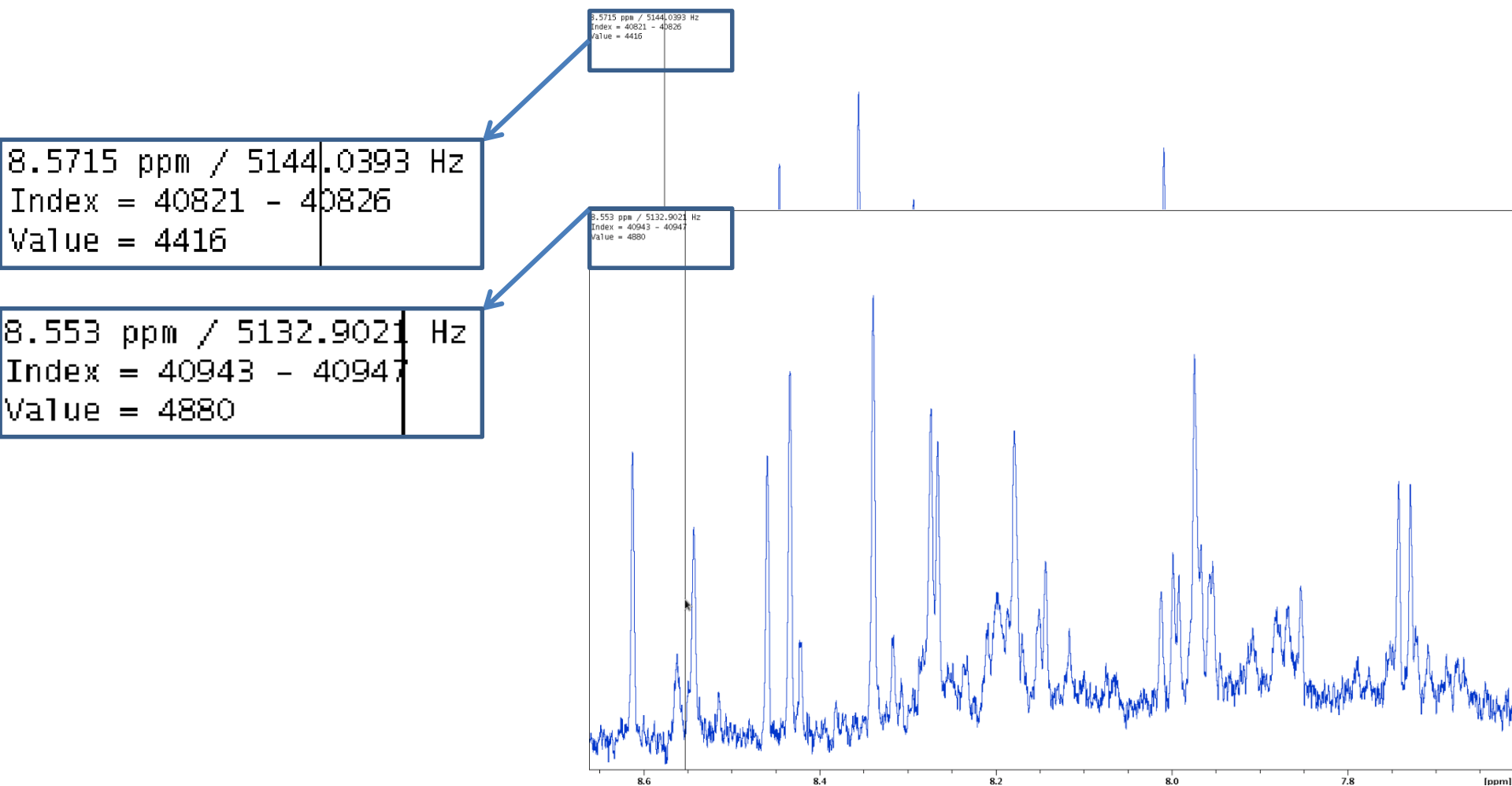




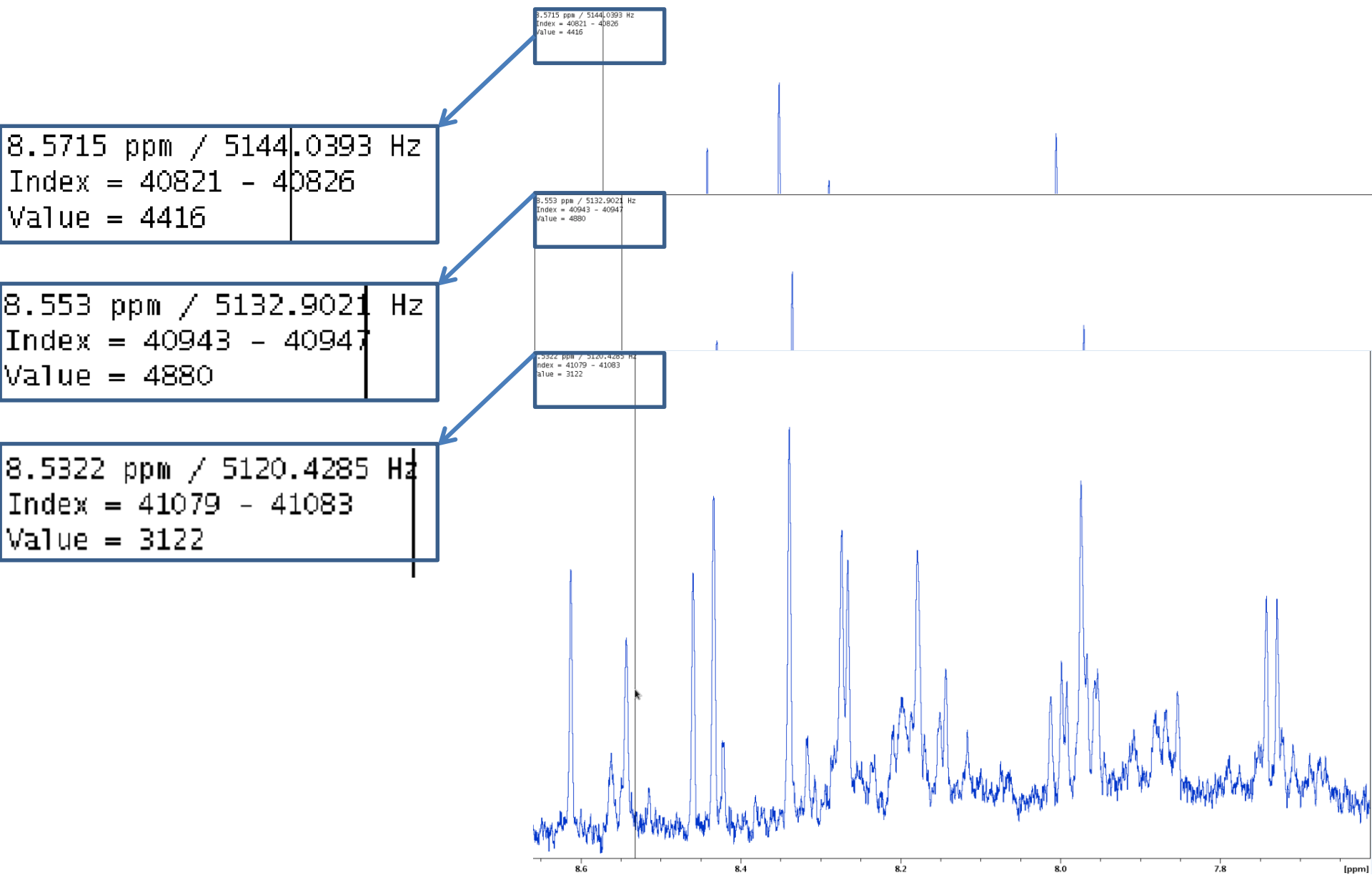
# Preparing a Pattern File



# Preparing a Pattern File



# Preparing a Pattern File



# Preparing a Pattern File

8.5715 ppm / 5144.0393 Hz  
Index = 40821 - 40826  
Value = 4416

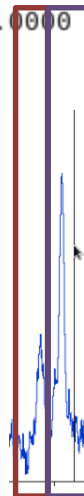
8.553 ppm / 5132.9021 Hz  
Index = 40943 - 40947  
Value = 4880

8.5322 ppm / 5120.4285 Hz  
Index = 41079 - 41083  
Value = 3122

0.0000	0.0000	8.270	8.259	0 AMP
0.0000	0.0000	8.279	8.270	0 ADP
0.0000	0.0000	8.344	8.330	0 aro11
0.0000	0.0000	8.389	8.378	0 aro12
0.0000	0.0000	8.427	8.417	0 NADP2
0.0000	0.0000	8.445	8.433	0 NAD2
0.0000	0.0000	8.464	8.454	0 formate
0.0000	0.0000	8.505	8.496	0 aro13
0.0000	0.0000	8.522	8.505	0 ATP
0.0000	0.0000	8.553	8.532	0 ADP
0.0000	0.0000	8.572	8.553	0 aro14
0.0000	0.0000	8.617	8.596	0 AMP
0.0000	0.0000	8.858	8.822	0 NADP+NAD8
0.0000	0.0000	9.125	9.000	0 NADP3
0.0000	0.0000	9.175	9.137	0 NAD9
0.0000	0.0000	9.301	9.291	0 NADP4
0.0000	0.0000	9.355	9.335	0 NAD10

aro14

ADP



# Pattern File Format

#	Data				
1	\$##DATE      The date in ddmmyy format e.g 150915				
2					
3	PATTERN      = Sample name and the type of metabolites				
4	GROUP      = The group you are working for				
5	DESCRIPTION = Any additional information				
6	AUTHOR      = Your name				
7	DIM      = 2 Leave it as 2				
8	ORIGIN      = 1 Leave it as 1				
9	ITEMS      = 11 Write the exact number of peaks you selected*				
10	0.0000	0.0000	0.6834	0.6751	0 Chol-18
11	0.0000	0.0000	1.0128	1.0064	0 Chol-19
12	0.0000	0.0000	1.2698	1.2362	0 TAA ?
13	0.0000	0.0000	2.3673	2.3608	0 TAA-1
14	0.0000	0.0000	2.4839	2.4581	0 =CH-CH2-CH=?
15	0.0000	0.0000	2.8184	2.7795	0 TAA-2
16	0.0000	0.0000	3.4995	3.4868	0 -N+(CH3)3
17	0.0000	0.0000	4.0191	4.0084	0 glyceryl-C3H (PC/PE)
18	0.0000	0.0000	4.1217	4.1115	0 LDL
19	0.0000	0.0000	4.1319	4.1217	0 glyceryl backbone CH2-1
20	0.0000	0.0000	4.2554	4.2461	0 glyceryl backbone CH2-2

# Pattern File Format

#	Data				
1	\$\$\$DATE 150915 <i>The date in <u>ddmmyy</u> format</i>				
2					
3	PATTERN = Plasma Antibiotics <i>Sample name and the type of metabolites</i>				
4	GROUP = <u>IGH</u> <i>The group you are working for</i>				
5	DESCRIPTION = Control <i>Any additional information</i>				
6	AUTHOR = A Researcher <i>Your name</i>				
7	DIM = 2 <i>Leave it as 2</i>				
8	ORIGIN = 1 <i>Leave it as 1</i>				
9	ITEMS = 11 <i>Write the exact number of peaks you selected*</i>				
10	0.0000	0.0000	0.6834	0.6751	0 <u>Chol</u> -18
11	0.0000	0.0000	1.0128	1.0064	0 <u>Chol</u> -19
12	0.0000	0.0000	1.2698	1.2362	0 <u>TAA</u> ?
13	0.0000	0.0000	2.3673	2.3608	0 <u>TAA</u> -1
14	0.0000	0.0000	2.4839	2.4581	0 =CH-CH2- <u>CH</u> =?
15	0.0000	0.0000	2.8184	2.7795	0 <u>TAA</u> -2
16	0.0000	0.0000	3.4995	3.4868	0 -N+(CH3)3
17	0.0000	0.0000	4.0191	4.0084	0 glyceryl-C3H (PC/PE)
18	0.0000	0.0000	4.1217	4.1115	0 <u>LDL</u>
19	0.0000	0.0000	4.1319	4.1217	0 <u>glyceryl</u> backbone CH2-1
20	0.0000	0.0000	4.2554	4.2461	0 <u>glyceryl</u> backbone CH2-2

- Always use plain text.
  - Never use a word processor (e.g MS Word, OpenOffice, etc).
  - If prepared on Windows always check you file on linux text editor (e.g nedit).
- Files prepared on Windows may introduce "<cr>" in your line. If this happens simply delete every <cr> and save the file before you proceed.

# Galaxy - TameNMR

**Galaxy**

Analyze DataWorkflowShared DataVisualizationHelpUser

Using 0 bytes

Tools

search tools

[Get Data](#)  
[Import Data](#)  
[Spectra Processing](#)  
[Data Preparation](#)  
[Plots](#)  
[Statistics](#)

**Workflows**  
All workflows

**tameNMR - tools for Analysis of METabolic NMR (test version)**

Configuring Galaxy »Installing Tools »

Galaxy is an open platform for supporting data intensive research. Galaxy is developed by The Galaxy Team with the support of many contributors.

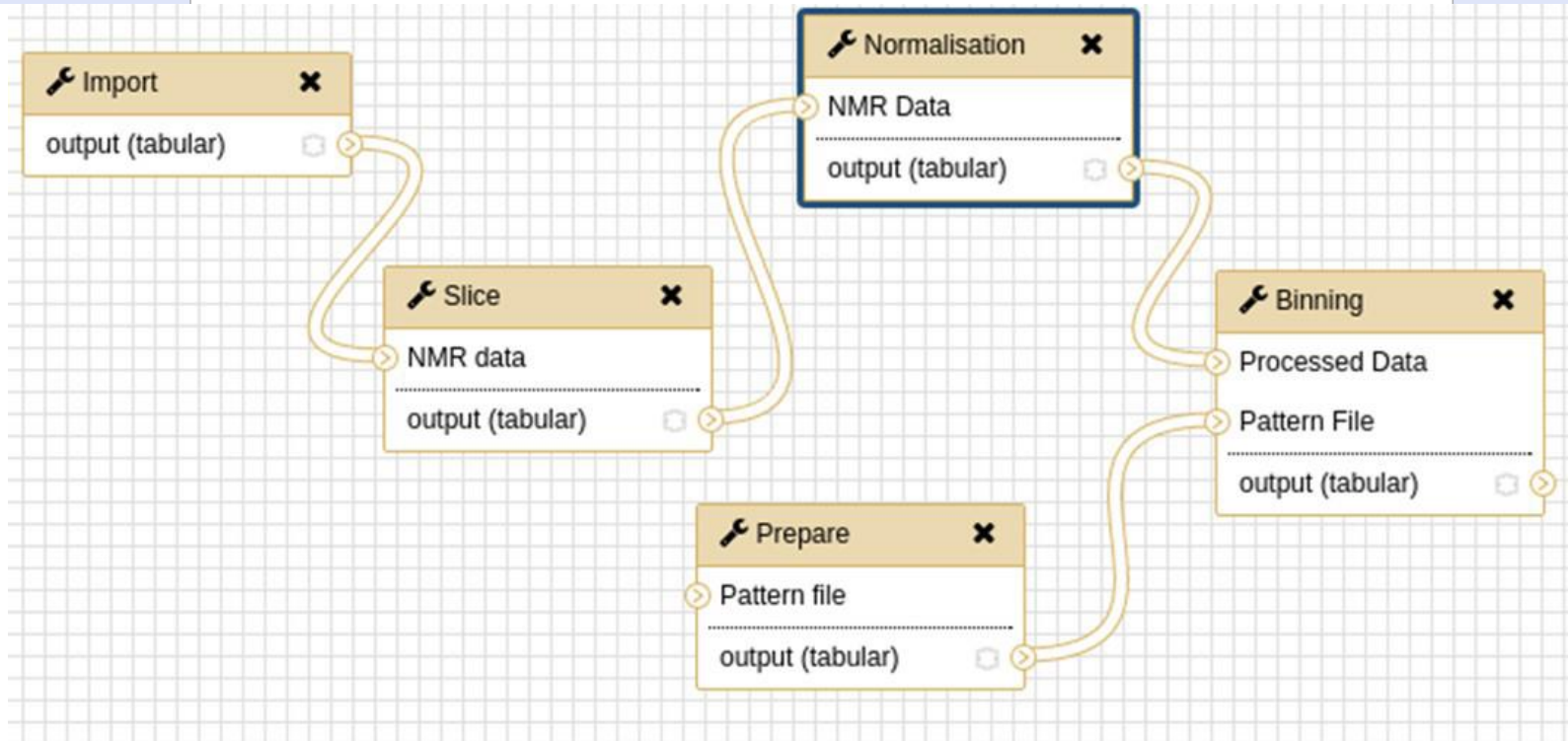
The Galaxy Project is supported in part by NHGRI, NSF, The Huck Institutes of the Life Sciences, The Institute for CyberScience at Penn State, and Johns Hopkins University.

History

search datasets

**Unnamed history**  
(empty)

This history is empty. You can [load your own data](#) or [get data from an external source](#)



# Galaxy - TameNMR

## 1. Import - Import of NMR data (from Bruker raw files)

Bruker to csv

## 2. Process Spectra

Normalisation

Peak Picking

Spectra alignment

Binning

## 3. Process Data

Scaling

Make factor template (for grouping observations)

## 4. Statistics - univariate and multivariate statistics

t-tests

one-way ANOVA

Principal component analysis (PCA)

Partial least squares discriminant analysis (PLS-DA)

## 5. Plots - various plotting tools for:

Raw NMR spectra


Quantiles of spectra

Significant bins ( $p$ -values from t-tests of ANOVA)

Significant bins (mean value comparison)



# TameNMR – Register & Login

 Analyze Data Workflow Shared Data Visualization Help User Using 0 bytes

Create account

**Email address:**


**Password:**

Strength

**Confirm password:**

**Public name:**

Your public name is an identifier that will be used to generate addresses for information you share publicly. Public names must be at least three characters in length and contain only lower-case letters, numbers, dots, underscores, and dashes (., \_, -).

 Analyze Data Workflow Shared Data Visualization Help User Using 0 bytes

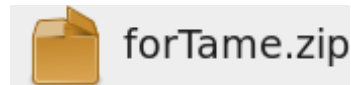
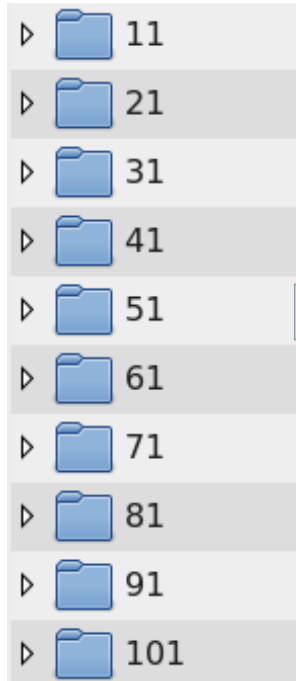
Login

**Username / Email Address:**

**Password:**

[Forgot password? Reset here](#)

# TameNMR – Data Formats



. A set of Bruker format Spectra can be zipped together for upload (do not zip dataset parent folder but individual experiment numbers)

. Alternatively prepare a table with tab separated columns (every spectrum in a different column, header containing spectra ID)

. Tab separated column formats must also be prepared for bin boundary **pattern** files (peak annotation) and sample groupings (for statistical analysis).

1	2	3	4
"ppm"	"A194"	"B195"	"C196"
9.99990639748	583.224970898215	49.6107431222747	-219.231228317496
9.99977543254	419.501182307945	-223.745293769119	-79.6887423671469
9.9996444676	357.159005369531	-370.219117690402	94.052768959037
9.99951350265	521.642853750682	-461.051418850098	502.15241976322
9.99938253771	605.491267953802	-396.936482237745	884.510165552195
9.99925157277	490.273113290677	-151.359092344189	928.059976069032
9.99912060783	403.868134336411	32.781835693021	768.74788144062
9.99898964288	383.933838911936	-27.7112639851076	710.943027841694
9.99885867794	253.859970154316	-194.36630021895	755.648063562432

The screenshot displays the Galaxy web interface. At the top, the 'Galaxy' logo is on the left, and navigation links for 'Analyze Data', 'Download Data', 'Create New Dataset', 'Help', and 'About' are in the center. The right corner shows a user profile icon and the text 'Using 90.8 MB'. The left sidebar contains a 'Tools' section with a search bar and a list of tool categories: 'Get Data', 'Annotate Data', 'Sample Processing', 'Data Visualization', 'File', 'Transformation & Manipulation', 'Data Integration', 'Data Analysis', and 'Data Archiving'. The main content area features the title 'tameNMR - tools for Analysis of METabolic NMR' with two buttons: 'Configure Galaxy' and 'Installing Tools'. Below this, a paragraph describes Galaxy as an open platform for data-intensive research, developed by The Galaxy Team. The right sidebar shows a 'History' section with a list of datasets, including 'tameNMR - tools for Analysis of METabolic NMR' and 'tameNMR - tools for Analysis of METabolic NMR'.

Import Spectra – Bruker data:  
<https://youtu.be/Fc2g5oIF6Jw>



Import peak boundaries – pattern file:

<https://youtu.be/wH2g4CDa2Dk>

# TameNMR – Data import

Galaxy

Analyze Data Workflow Shared Data Visualization Help User

Using 1.9 GB

Tools

search tool

Get Data

Upload File

Import Data

Spectra Proc

Data Prepara

Plots

Trypanosom

Statistics

Trypanosom

Workflows

All workflow

Download from web or upload from disk

Regular Composite

You added 1 file(s) to the queue. Add more files or click 'Start' to proceed.

Name	Size	Type	Genome	Settings	Status
forTame.zip	7.6 MB	Auto-detect	unspecified (?)		

Type (set all): Auto-detect

Genome (set all): unspecified (?)

Choose local file Choose FTP file Paste/Fetch data Pause Reset Start Close

inc\_for\_pat\_check1.tsv

.Upload spectra and annotation *via* drag and drop



# TameNMR – Data import

The screenshot displays the Galaxy web interface. A modal window titled "Download from web or upload from disk" is open, showing the "Regular" tab. Inside the modal, a table lists the imported data:

Name	Size	Type	Genome	Settings	Status
forTame.zip	7.6 MB	Auto-detect	unspecified (?)		100%

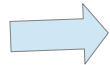
Below the table, there are filters for "Type (set all):" and "Genome (set all):". At the bottom of the modal, there are buttons for "Choose local file", "Choose FTP file", "Paste/Fetch data", "Pause", and "Reset".

In the background, the Galaxy interface shows a sidebar with various tools and a "History" panel on the right. The "History" panel lists datasets, including "Unnamed history" and "708: forTame.zip". A red arrow points from the "708: forTame.zip" entry in the history panel to the "forTame.zip" entry in the modal window's table.

.Should appear in right hand browser

# TameNMR – Data import

0.0000	0.0000	8.270	8.259	0 AMP
0.0000	0.0000	8.279	8.270	0 ADP
0.0000	0.0000	8.344	8.330	0 aro11
0.0000	0.0000	8.389	8.378	0 aro12
0.0000	0.0000	8.427	8.417	0 NADP2
0.0000	0.0000	8.445	8.433	0 NAD2
0.0000	0.0000	8.464	8.454	0 formate
0.0000	0.0000	8.505	8.496	0 aro13
0.0000	0.0000	8.522	8.505	0 ATP
0.0000	0.0000	8.549	8.537	0 ADP
0.0000	0.0000	8.570	8.560	0 aro14
0.0000	0.0000	8.617	8.596	0 AMP
0.0000	0.0000	8.858	8.822	0 NADP+NAD8



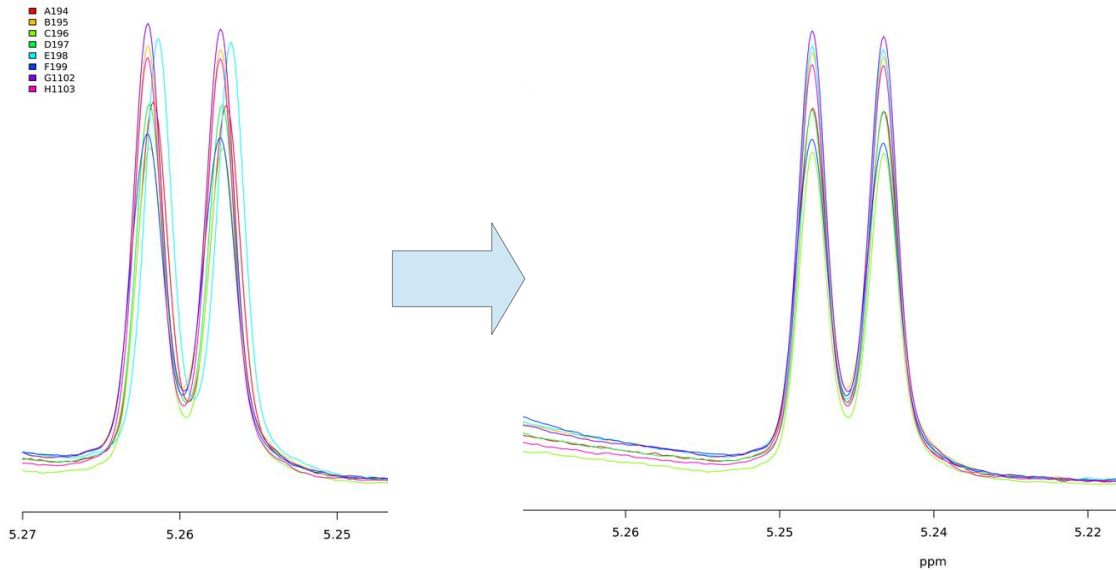
The screenshot shows the Galaxy web interface. On the left is a sidebar with tool categories: Get Data, Import Data, Spectra Processing, Data Preparation, Plots, Trypanosoma VAP, Statistics, and Trypanosoma vapper (official tool). The 'Import Data' section is expanded, showing 'Import Bruker NMR data' and 'Prepare pattern file'. The main panel displays the 'Import Bruker NMR data (Galaxy Version 0.0.1)' tool configuration. The 'NMR data source' is set to 'Data'. The 'Bruker Experiment' dropdown shows '708: forTame.zip'. An 'Execute' button is visible. Below the configuration, a description states: 'This tool converts a Bruker experiment files to a format used internally within tameNMR. It requires a zip file uploaded through the upload tool to your account. The file should contain a set of Bruker NMR experiments without the parent directory. To make the zip file you can enter your Bruker experiment folder containing folders with spectra(e.g. 10, 20, 30 etc.), select all folders that you want to add to zip file, right-click, choose compress, select zip format and click OK. The resulting file can then be uploaded and imported using this tool.' On the right, the 'History' panel shows a list of datasets: '708: forTame.zip', '707: NMR Plot', '705: Imported NMR data', '662: NMR Plot', '661: Imported NMR data', '657: NMR Plot', and '556: NMR Plot'. Each entry has icons for viewing, editing, and deleting.

loaded

- Import the bruker data to unzip and tabulate (column per spectrum).
- Import from spreadsheet/text file the **Pattern** or bin boundaries

# TameNMR – Process Spectra

## Alignment

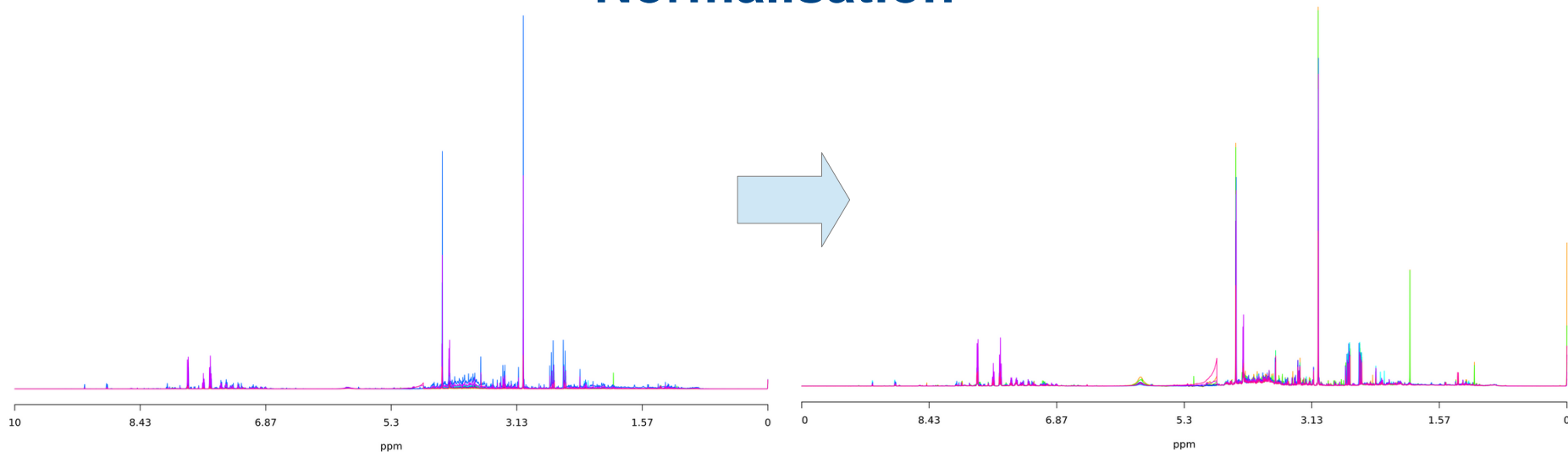


Align to different reference peak

Data normalisation may be applied

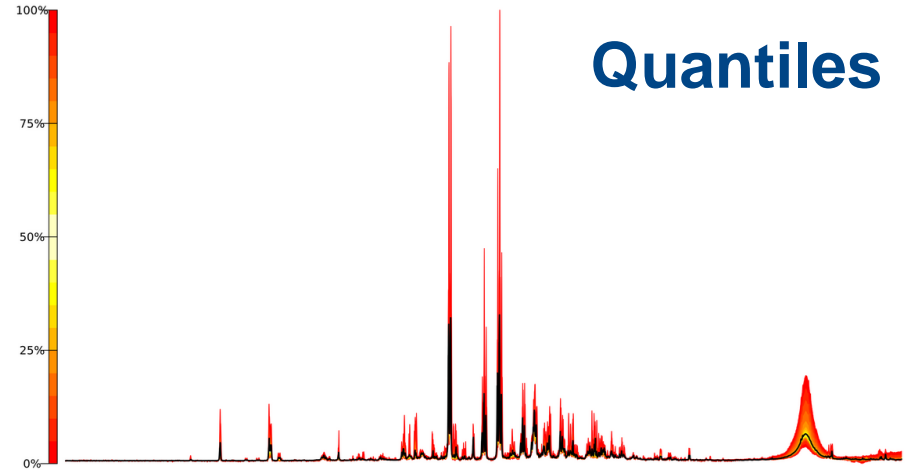
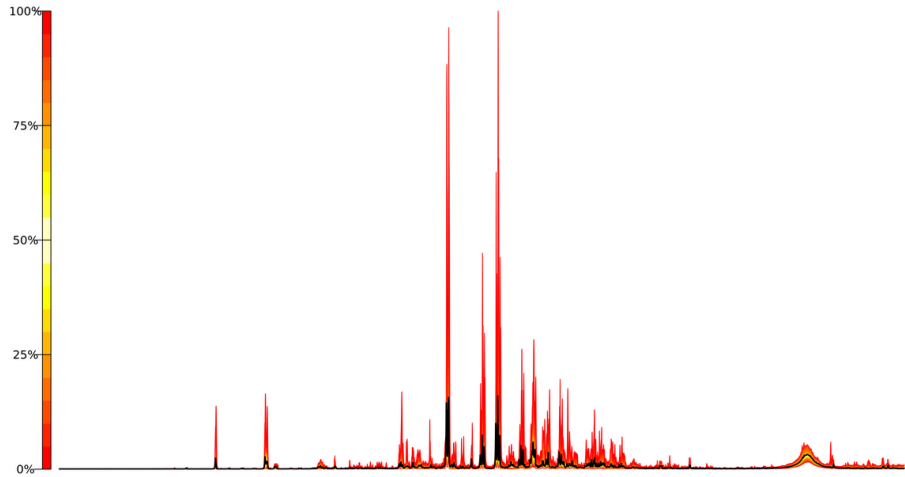
- Peak picking function enables
- Binning spectra using predefined

## Normalisation





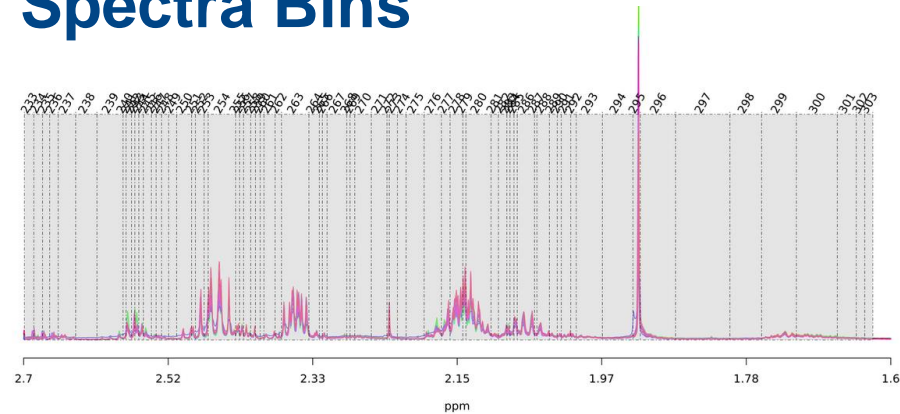
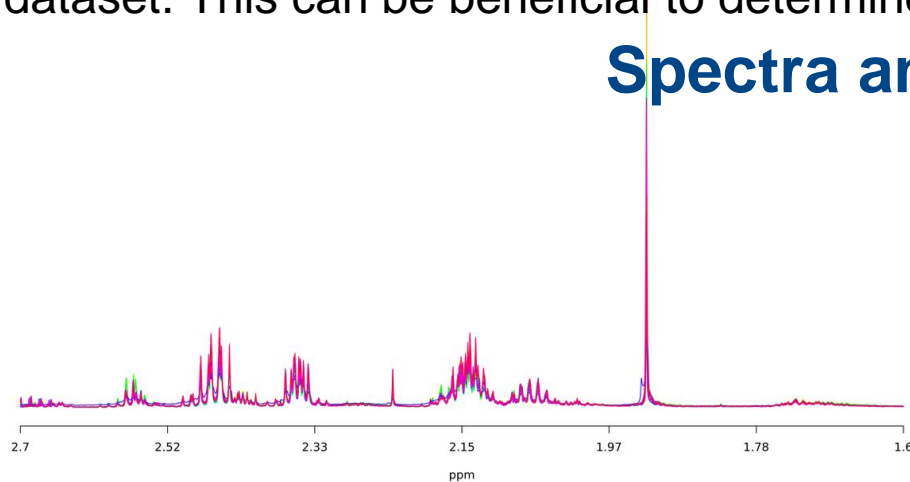
# TameNMR – Process Spectra



Quantiles

Quantile plot of the spectra can show median (black) and variance for a particular dataset. This can be beneficial to determine normalisation efficacy


## Spectra and Spectra Bins



Quality of overlay of bins (peak boundaries) with spectra is key to quality of data analysis. This function was a driving factor for generating this toolkit.



# TameNMR – spectra slicing

 Galaxy

Analyze DataWorkflowShared DataVisualizationHelpUser



Using 274.5 MB

Tools

search tools

**Get Data**  
**Import Data**  
**Spectra Processing**  
    [Slice NMR spectra](#)  
    [Normalisation](#)  
    [Peak picking](#)  
    [Spectra alignment](#)  
    [Binning \(Bucketing\)](#)  
**Data Preparation**  
**Statistics**  
**Plots**  
  
**Workflows**  
    [All workflows](#)

**Slice NMR spectra (Galaxy Version 0.0.1)** Options

**NMR data**  
  18: Sliced Data

**Retain ppm**  
10-0




**Remove water signal**




This tool retains selected regions of the spectra and removes the rest. The regions should be entered in ppm and separated by commas. Ex: "10-0" will remove any spectral regions outside of the range 0 to 10 ppm.

History


search datasets

**Unnamed history**  
2 shown, 16 [deleted](#)  
274.45 MB

**18: Sliced Data**   

**1: Imported NMR data**   

# TameNMR - Normalisation



Analyze DataWorkflowShared DataVisualizationHelpUser




Using 310.1 MB

Tools

search tools

**Get Data**  
**Import Data**  
**Spectra Processing**  
    [Slice NMR spectra](#)  
    [Normalisation](#)  
    [Peak picking](#)  
    [Spectra alignment](#)  
    [Binning \(Bucketing\)](#)  
**Data Preparation**  
**Statistics**  
**Plots**  
  
**Workflows**  
    [All workflows](#)

Normalisation (Galaxy Version 0.0.1) Options



19: Normalised Data

Normalisation method

PQN

Execute

History

search datasets


Unnamed history  
3 shown, 16 deleted  
310.14 MB

19: Normalised Data

18: Sliced Data

1: Imported NMR data

# TameNMR – Binning

 Galaxy

Analyze DataWorkflowShared DataVisualizationHelpUser

Using 310.3 MB

Tools

search tools

**Get Data**  
[Upload File](#) from your computer

**Import Data**  
[Import](#) Bruker NMR data  
[Prepare](#) pattern file




**Spectra Processing**  
[Slice](#) NMR spectra  
[Normalisation](#)  
[Peak picking](#)  
[Spectra alignment](#)  
[Binning](#) (Bucketing)

**Data Preparation**  
[Statistics](#)  
[Plots](#)

**Workflows**  
▪ [All workflows](#)

**Binning (Bucketing)** (Galaxy Version 0.0.1) Options




**Processed Data**

 22: Binned Spectra

**Method**

Pattern

**Pattern File**




 21: Pattern




✓ Execute




History




search datasets




Unnamed history  
5 shown, 17 deleted  
310.28 MB

**22: Binned Spectra**

**21: Pattern**

**19: Normalised Data**

**18: Sliced Data**

**1: Imported NMR data**

# TameNMR - Workflows

## Your workflows

[+ Create new workflow](#)[↑ Upload or import workflow](#)

Name	# of Steps
NMR_Standard_uniformBins ▾	4
NMR_Standard ▾	5


## Workflows shared with you by others

No workflows have been shared with you.

## Other options

[Configure your workflow menu](#)

# TameNMR - Workflows

 Galaxy

Analyze DataWorkflowShared DataVisualizationHelpUser

Using 310.3 MB

Tools

search tools

[Get Data](#)[Import Data](#)[Spectra Processing](#)[Data Preparation](#)[Statistics](#)[Plots](#)

Workflows

- All workflows

Running workflow "NMR\_Standard"Expand AllCollapse

NMR data import with water signal removal, PQN normalisation and pattern based binning

Step 1: Import (version 0.0.1)

Bruker Experiment

File	Size	Date
<input checked="" type="checkbox"/> CPMG_exp.zip	26.4 MB	10/21/2016 10:43:44 am

This Galaxy server allows you to upload files via FTP. To upload some files, log in to the FTP server at **None** using your Galaxy credentials (email address and password).

Step 2: Prepare (version 0.0.1)

Pattern file

21: Pattern

Type of pattern file

Bruker pattern file

Step 3: Slice (version 0.0.1)

Step 4: Normalisation (version 0.0.1)

Step 5: Binning (version 0.0.1)

☐ Send results to a new history

Run workflow

History

search datasets

Unnamed history

5 shown, 17 deleted

310.28 MB

22: Binned Spectra


21: Pattern

19: Normalised Data

18: Sliced Data

1: Imported NMR data

# TameNMR - workflows

 Galaxy

Analyze DataWorkflowShared DataVisualizationHelpUser

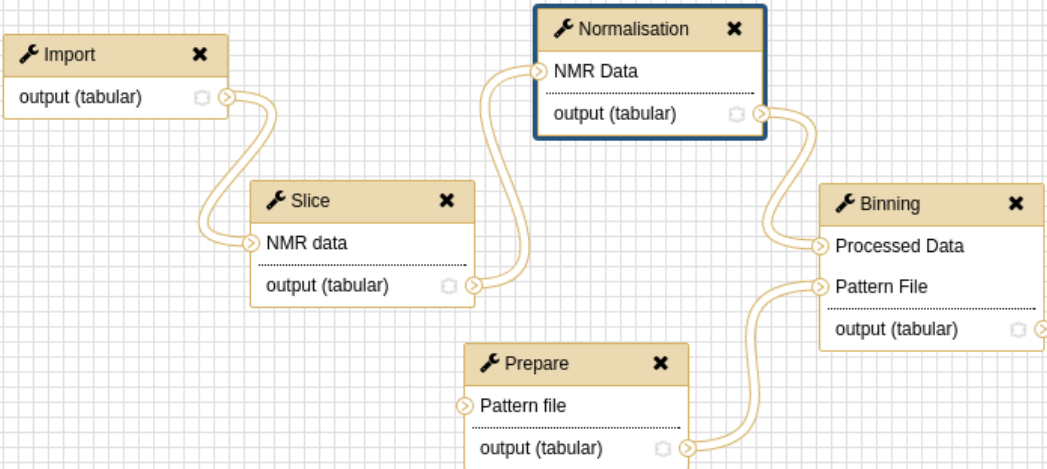
Using 310.3 MB

Tools

search tools

[Inputs](#)  
[Get Data](#)  
[Import Data](#)  
[Spectra Processing](#)  
[Data Preparation](#)  
[Statistics](#)  
[Plots](#)  
[Workflows](#)

Workflow Canvas | NMR\_Standard



```
graph LR; Import[Import] --> Slice[Slice]; Slice --> Prepare[Prepare]; Prepare --> Normalisation[Normalisation]; Normalisation --> Binning[Binning];
```

Details

**Normalisation** (Galaxy Version 0.0.1)

**NMR Data**  
Data input 'input' (data)

**Normalisation method**  
PQN

**Annotation / Notes**  

Add an annotation or note for this step. It will be shown with the workflow.

**Email notification**  

Yes No

  
An email notification will be sent when the job has completed.

**Output cleanup**  

Yes No

  
Delete intermediate outputs if they are not used as input for another job.

[Configure Output: 'output'](#)



# Acknowledgements

## Liverpool Metabolomics beta testers:

Rudi Grosman

Dr Eva Caamaño-Gutiérrez (CBF)

Adika Sen

Michelle Tan

Dan Sadler

Nicola Beesley

Alan Reynolds

Yetunde Adegbite

Thomas Leather

Zain Ghanameh

Mattia Scalibrin

Brendan Norman

Andrew Davison



## Technology Directorate:

Dr Duncan Robertson

Julie Boileau



## Liverpool Computational

### Biology (CBF):

Prof Andy Jones

Dr Arturas Grauslys



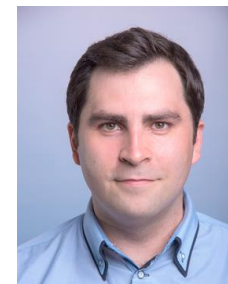
## Funding:

BBSRC TDRF2 call  
(BB/M020282/1)



 @LivUniNMR

 @LivUniCBF



E: [mphelan@liverpool.ac.uk](mailto:mphelan@liverpool.ac.uk)

Download from git-hub:

<https://github.com/PGB-LIV/tameNMR>



tameNMR Protocols/guide:

<https://sites.google.com/view/amenmr>



tameNMR mailing list:

<https://forms.gle/q8VS2rHT479dNow27>



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BB/M020282/1

tameNMR tutorials:

<https://youtube.com/channel/UCw92VXikB44MVklWW24p2fA>



CCPN tutorials:

<https://youtube.com/channel/UCKyPsbC0mgaXAn03Owah50w>



tameNMR mailing list:

<https://forms.gle/XKfiVPuT1RiURQ7a7>

