

NMR Metabolomics via CCPN: Integrating 1D and 2D NMR from repositories and standard libraries

<https://www.ccpn.ac.uk>

<https://www.ccpn.ac.uk/forums>

CCPN

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Installation

Information about downloading and installing CcpNmr Analysis V3

Installation on Mac or Linux
How to download and install CcpNmr Analysis V3 for Mac or Linux

Installing Updates
How to keep CcpNmr Analysis updated with all the latest Updates

CCPN

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 3. Analysing 2D NMR via Collaborative Computing Project for NMR (CCPN). This includes download of 2D NMR standards from BMRB (Biomolecular Resonance Bank)/ HMDB and overlay with CCPN metabolite library.

How do we verify metabolites?

2D NMR

Homonuclear

Heteronuclear

Spiking samples

Orthologous method:

Mass Spectrometry

Infrared Spectroscopy

Heteronuclear Two-Dimensional NMR

Advantages:

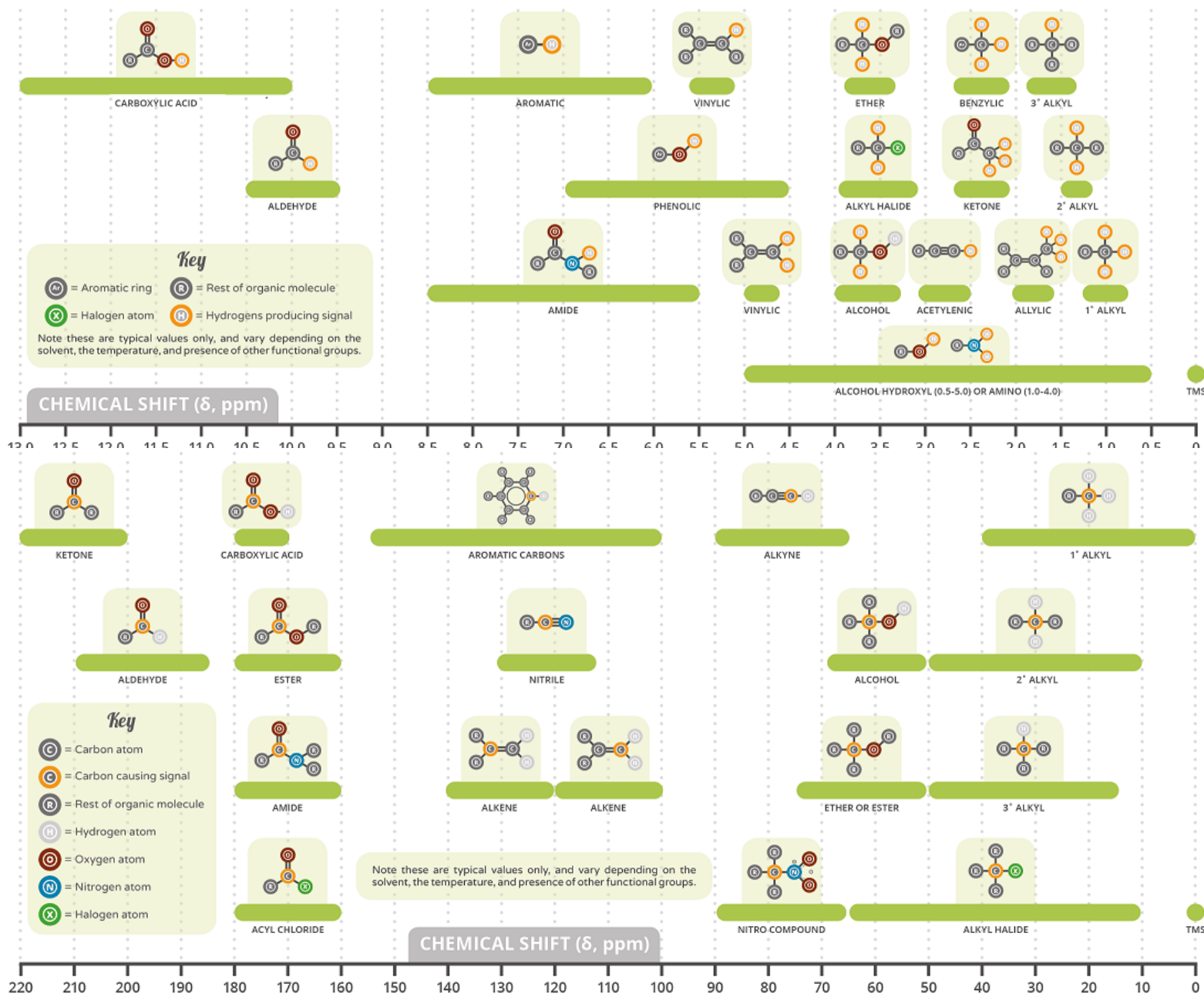
- Additional Dimension – reduces Ambiguity
- Decoupling reduces complexity
- ^{13}C chemical shift range more informative than ^1H
- ^{13}C can be used to monitor metabolic flux

Limitations:

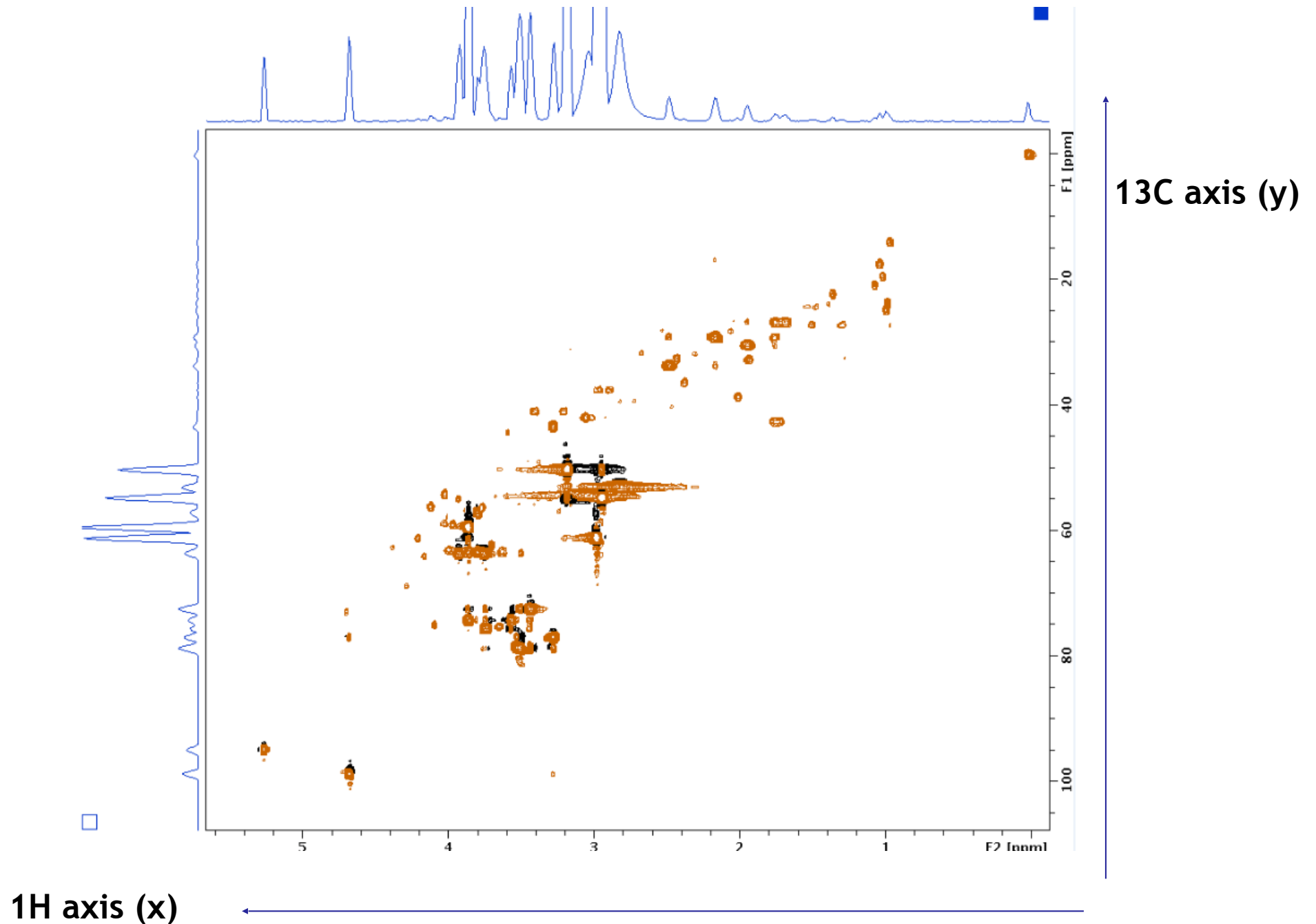
- Sensitivity Reduced
 - (^{13}C only 1.1% natural abundance)
- Increased time (collect multiple spectra to build up 2D)
- Less standard metabolite spectra available
- Does not integrate easily metabolomics tools

Chignola *et al* The CCPN Metabolomics Project: a fast protocol for metabolite identification by 2D-NMR. *Bioinformatics*. 2011 Jan 6; 27(6): 885-886

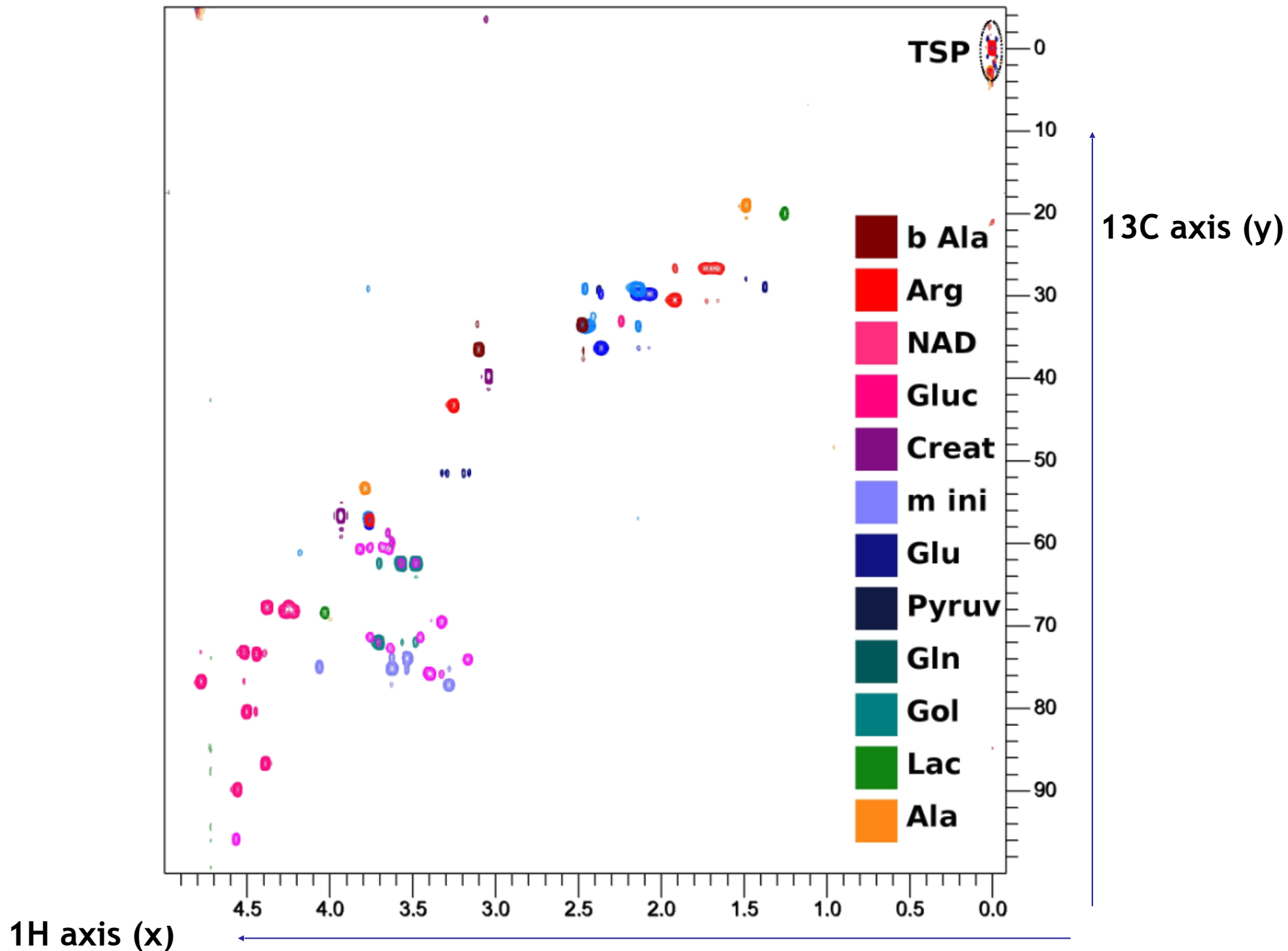
Heteronuclear Two-Dimensional NMR



How do we verify metabolites?

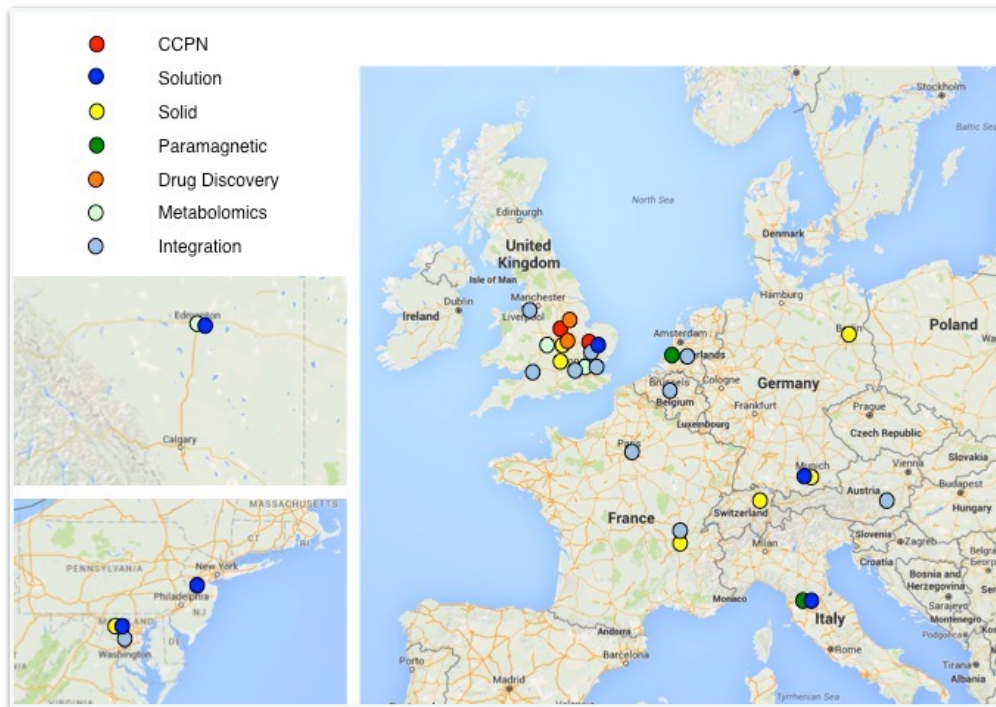


How do we verify metabolites?



CcpNmr Analysis version 3 software

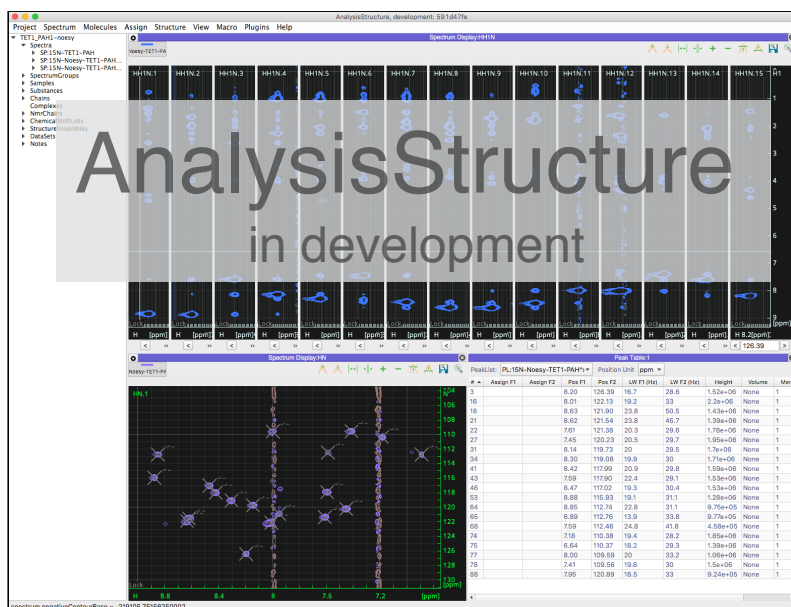
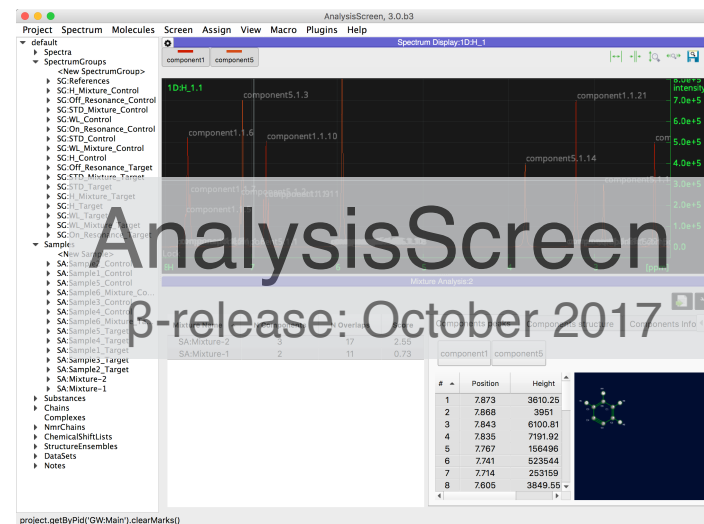
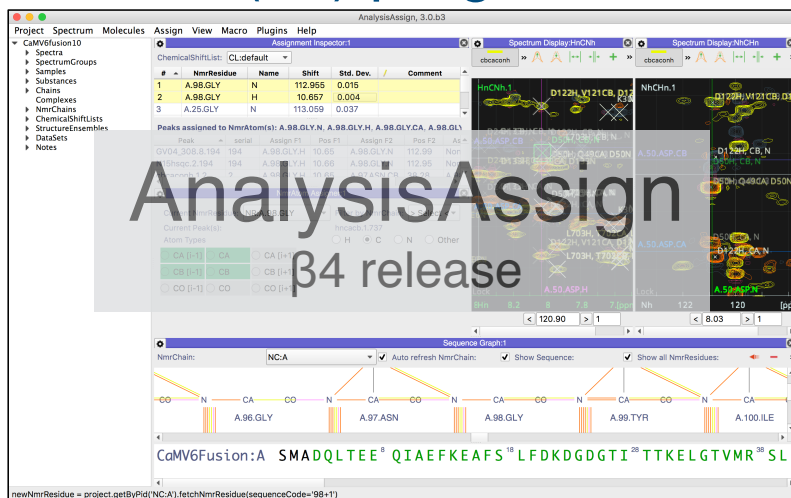
- Collaborative Computational Project for NMR (CCPN): exists since 2000
- MRC funded partnership (28 partners) network (2013-2016, 2016-2019)



- Support for software development, promoting best practices, knowledge sharing and collaboration

CcpNmr Analysis version 3 software

Suite of '4' (+1) programs:



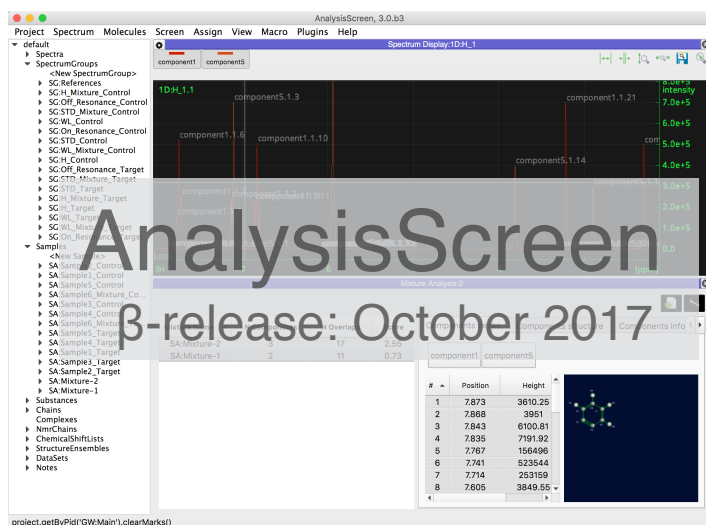
CcpNmr AnalysisAssign / MetaBonomics

Interface for nD assignment and data analysis:

- Drag and drop
- Adaptable and Customisable
- Flexible (easy python macro's)
- Scientific (e.g. Numpy, Scipy libraries)
- Fully V2 compatible (automatic conversion)
- Fully NEF compatible (import/export)
- Sparky importer
- SVG/PDF exporter for high quality plots

CcpNmr version 3 software

- AnalysisScreen: interface for NMR-based small-molecule screening
- AnalysisMetabolomics: interface for NMR-based metabolomics
- Extensive 1D capabilities (and nD of course) → also suitable for other small molecule NMR applications!
- Internal analysis/processing routines that function as 'pipes'
- Ability for complex operations, such as PCA and other multi-variate methods



AnalysisScreen
β-release: October 2017



AnalysisMetabolomics
α-release

CCPN Assign Demonstration

Lets visualise some 2D spectra from the metabolights repository (MTBLS626) using CCPN analysis

→ go to www.ebi.ac.uk/metabolights/MTBLS626

→ check study protocols tab (are there 2D spectra described in the NMR assay)
→ yes!

→ go to files tab (download m_a_i_s_ files as described in part 1 in order to check what spectra to download)

→ we selected:

→ download to zip

CAFLA 105EV1 2D

CAFLA 105EV2 2D

CAFLA 105EV3 2D

CAFLA 231EV1 2D

CAFLA 231EV2 2D

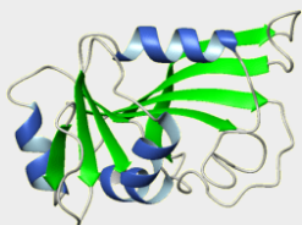
CAFLA 231EV3 2D

→ use CCPN assign to visualise spectra



Biological Magnetic Resonance Data Bank

A Repository for Data from NMR Spectroscopy on Proteins, Peptides, Nucleic Acids, and other Biomolecules



Google Custom Search



Home

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▸ Search archive

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▸ NMR Statistics

▸ Spectroscopists' Corner

▸ Programmers' Corner

▾ Metabolomics

Metabolomics Home

Standard Compounds

NMR Peaks Query

Molecular Mass Calculator

Find Formula/Molecule by Mass

Heuristically Determined

Formula by Mass

Atom Label Assignment Tool

using InChI String (ALATIS)

Server

Metabolomics Websites

Bulk Archives

Data Upload

Data policy

www.bmrwisc.edu/#menu metabolomics body

Instant entry access:

Searches all entries on many criteria: Title, Author, Entity, Organism, Database code, etc. Hover over a result for more information.

Search macromolecule database

If you have a query you would like to run on the BMRB database, please e-mail bmrhelp@bmrwisc.edu

	Field	Value to search for	Display
④	Entry ID (entry or accession number)	<input type="text"/>	<input checked="" type="checkbox"/>
④ ④ ④ ④ ④	<input type="text"/> PDB <input type="text"/> ID	<input type="text"/>	<input type="checkbox"/>
④ ④	Title	<input type="text"/>	<input type="checkbox"/>
④ ④	Author (family name)	<input type="text"/>	<input type="checkbox"/>
④ ④ ④	Molecule name	<input type="text"/>	<input type="checkbox"/>

Output ☒ HTML ☐ CSV ☐ inline

Search

Clear

[Restrictions Search](#)

[Metabolomics Search](#)

[Advanced Search](#)

[Help](#)

Deposit Data: [ADIT-NMR data deposition system](#).

Please look at the [data accepted](#) before depositing.

CS-Rosetta server.

Submit your chemical shifts to run CS-Rosetta.

BMRB API server and documentation.

Access BMRB data programmatically.

NMR Data Visualizations

New: **BMRB data visualizations in Python:** download from [GitHub](#) or try in a [Jupyter notebook](#)

RBMRB Visualizations



BMRB Data access

- Entry access

Specify Entry:

CCPN Assign Demonstration

- 1 – getting started & Importing Spectra
- 2 – creating a stacked plot (optional)
- 2a – rename via python
- 3 -printing pdf (optional)
- 4 – pipeline processing (optional)
- 5 – PCA (optional)

CcpNMR (CCPN) Tutorials:

[https://youtube.com/channel/
UCKyPsbC0mgaXAn03Owah50w](https://youtube.com/channel/UCKyPsbC0mgaXAn03Owah50w)

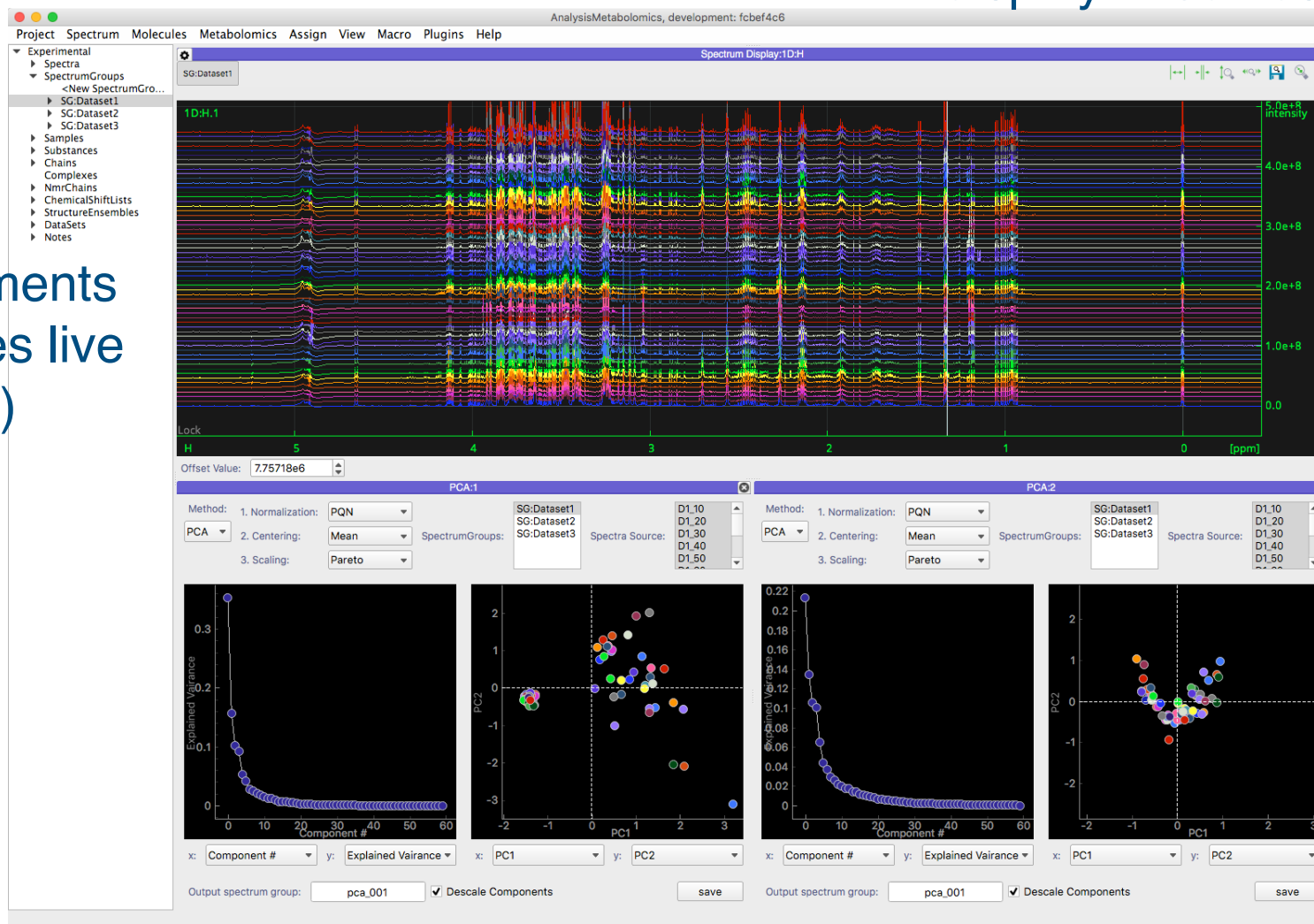


CcpNmr AnalysisMetabolomics

‘Modules’ contain the functionalities to display data

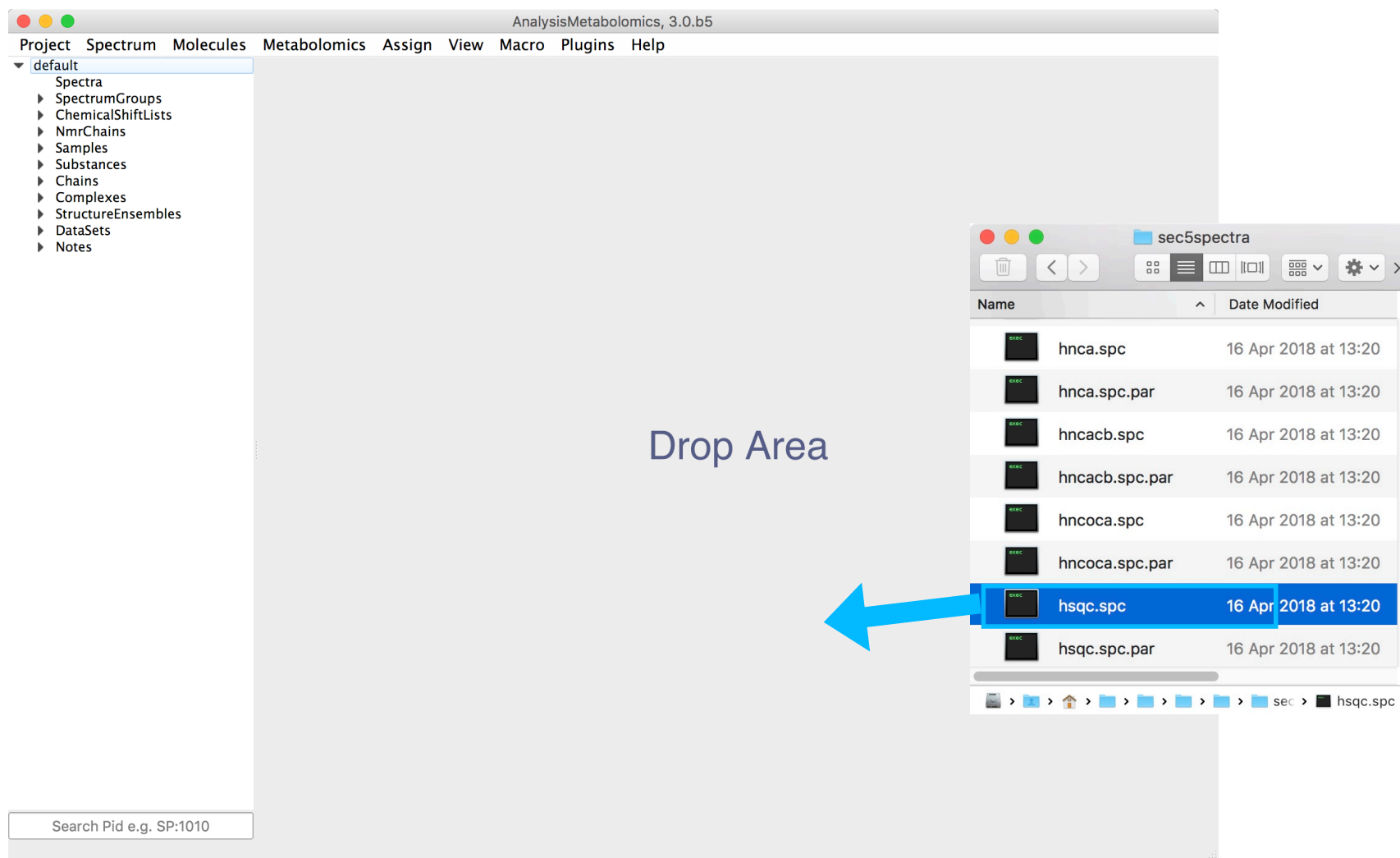
display ‘Modules’ (spectra)

data elements
(properties live
here)



PCA

CcpNmr AnalysisMetabolomics



CcpNmr AnalysisMetabolomics

AnalysisMetabolomics, 3.0.b5

Project Spectrum Molecules Metabolomics Assign View Macro Plugins Help

- ▼ default
 - Spectra
 - ▶ SpectrumGroups
 - ▶ ChemicalShiftLists
 - ▶ NmrChains
 - ▶ Samples
 - ▶ Substances
 - ▶ Chains
 - ▶ Complexes
 - ▶ StructureEnsembles
 - ▶ DataSets
 - ▶ Notes

←

	B	C	D	E	F	G	H	I	J	K	L	M	N
	substanceName	spectrumPath	spectrumGroupName	experimentType	comment	smiles	synonyms	molecularMass	atomCount	hBondAcceptorCount	hBondDonorCount	bondCount	ringCount
1	component1	component1	References	H	bi.ac.uk/chebi/searchId.do?chebiId=123456	C1=CC=CC=C1	RANDOM_NAME_-1,2-didehydrobenzene	185.00	6	3	3	3	1
2	component2	component2	References	H	bi.ac.uk/chebi/searchId.do?chebiId=123457	COC1=CC=CC=C1	DOM_NAME_methoxycyclohexa-1,3-dien-5-yl	190.00	8	2	3	4	1
3	component3	component3	References	H	bi.ac.uk/chebi/searchId.do?chebiId=123458	CC[NH3+]	RANDOM_NAME_ethylaminium	144.00	6	1	3	4	1
4	component4	component4	References	H	ssionid=64B6AB2667E275BC	CC(O)CC(O)=O	RANDOM_NAME_3-hydroxybutyric acid	190.00	7	1	3	3	1
5	component5	component5	References	H	bi.ac.uk/chebi/searchId.do?chebiId=123459	CC[NH3+]	RANDOM_NAME_mevalonic acid	185.00	6	1	3	3	1

Substances Samples_Control Samples_Target +

Search Pid e.g. SP:1010

Load from excel spreadsheets

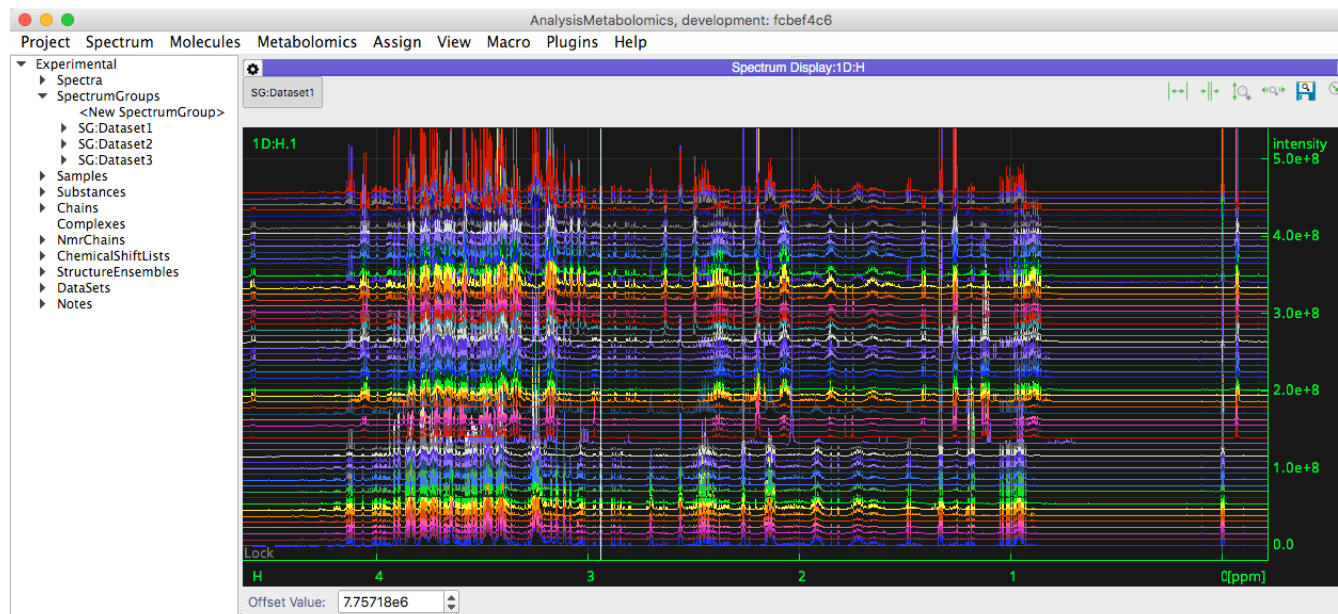
CcpNmr AnalysisMetabolomics



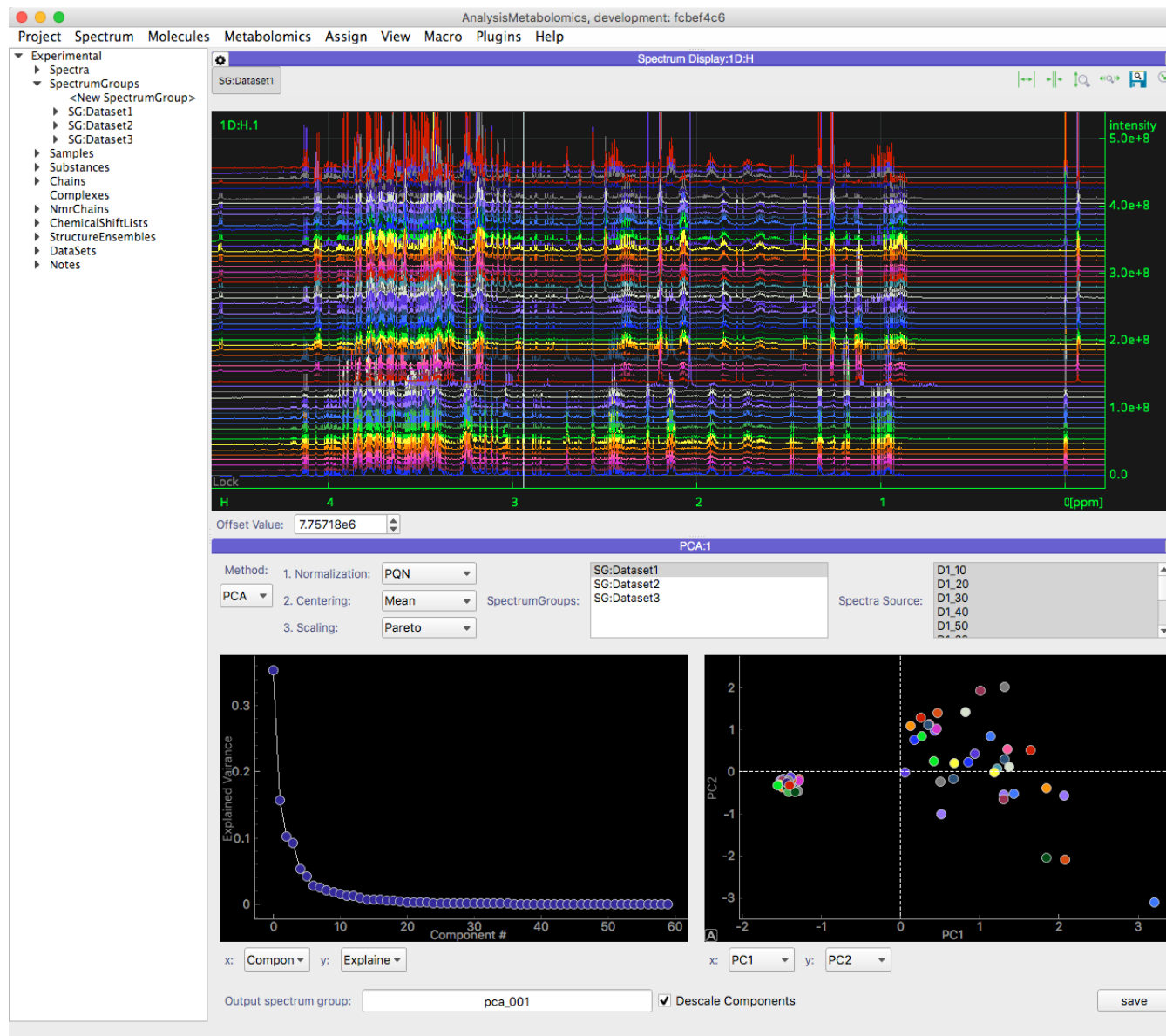
1D's

2D (nD)

CcpNmr AnalysisMetabolomics



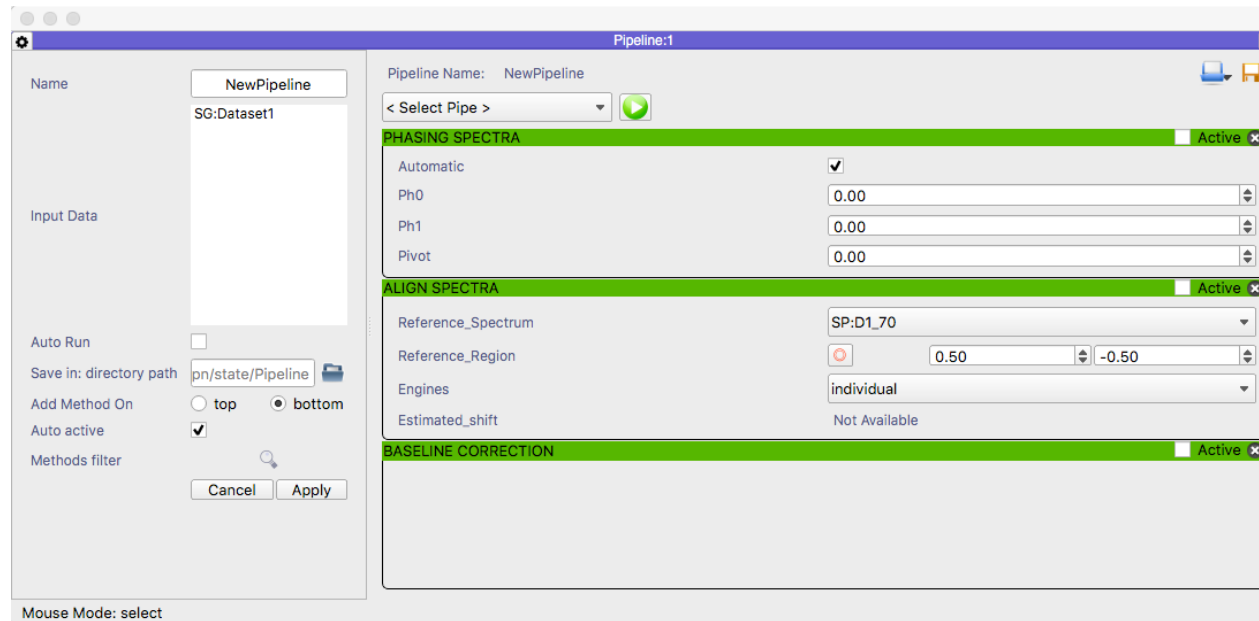
CcpNmr AnalysisMetabolomics



PCA

CcpNmr AnalysisMetabolomics

Processing pipes:
flexible way for data processing and analysis

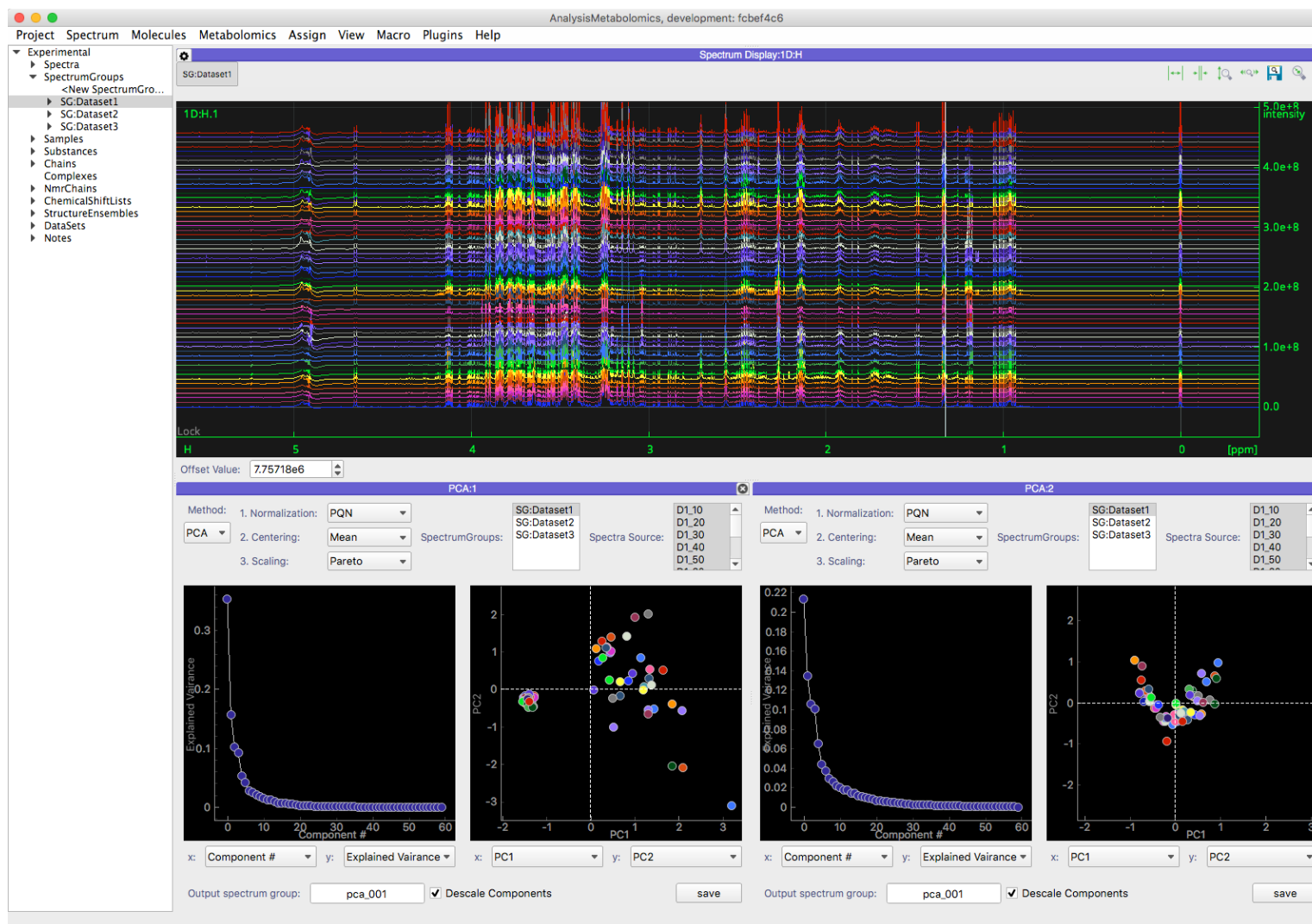


Automatic phasing

Aligning spectra

Baseline correction

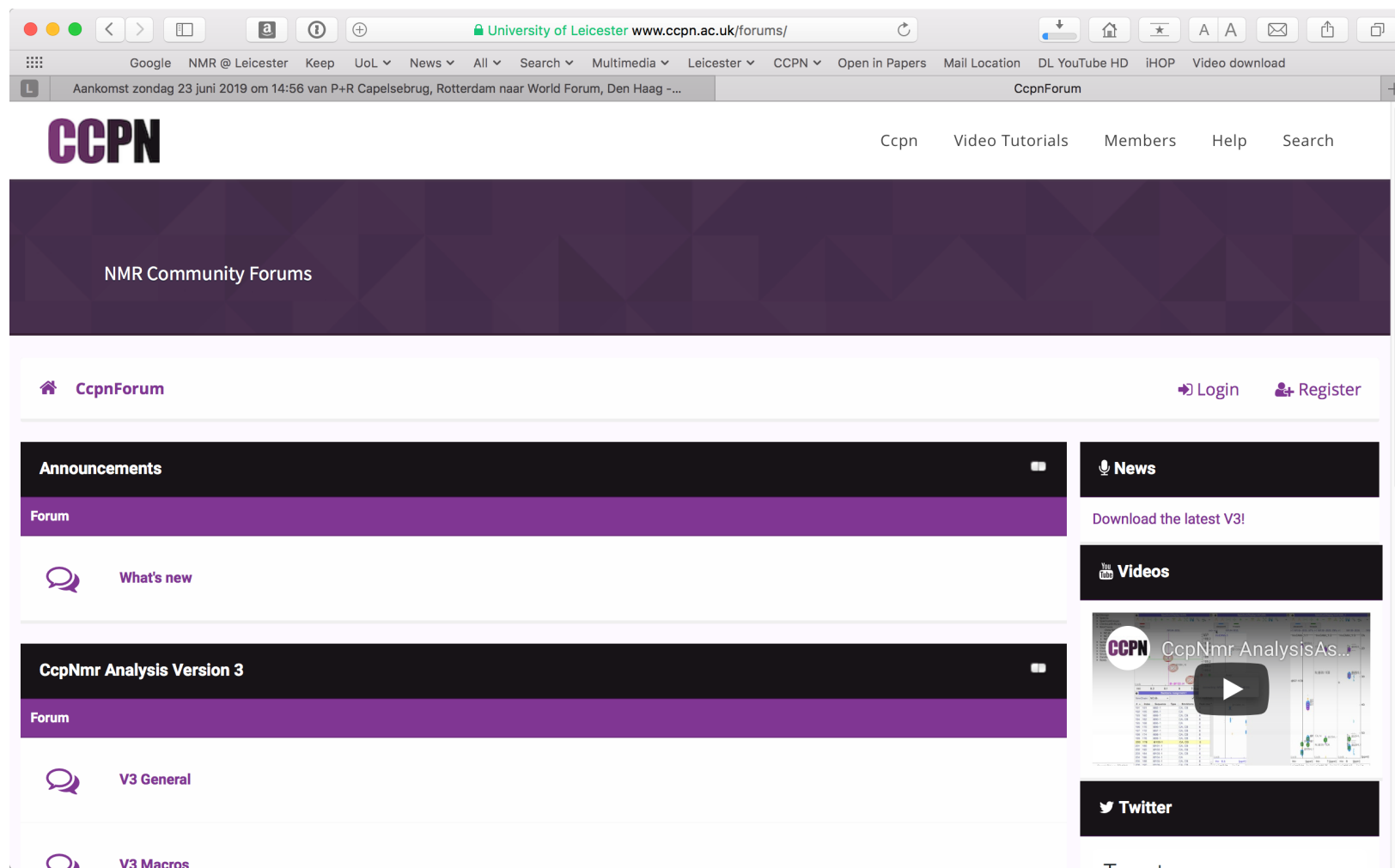
CcpNmr AnalysisMetabolomics



PCA (before)

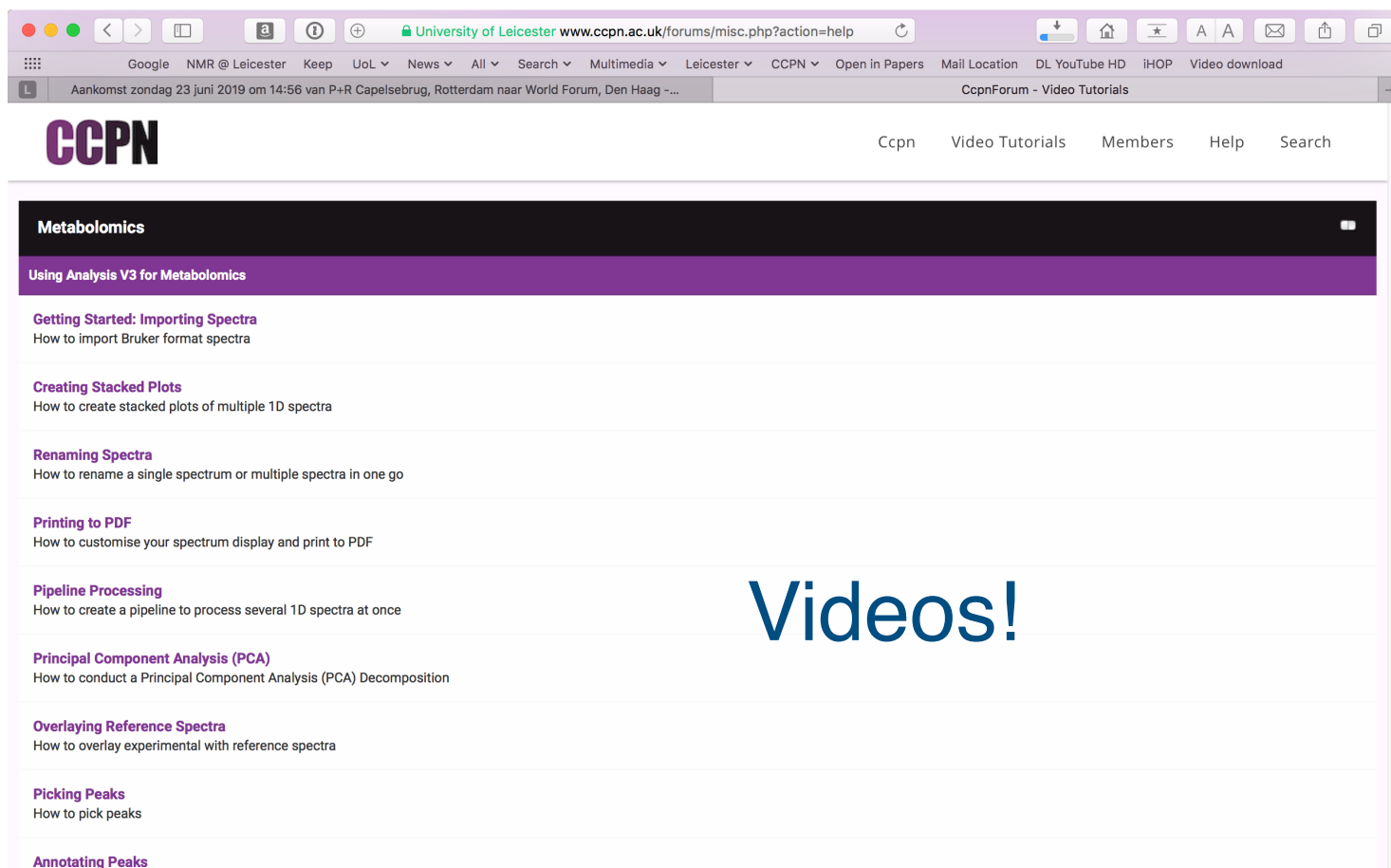
PCA (after)

CcpNmr forum



www.ccpn.ac.uk/forums

CcpNmr forum



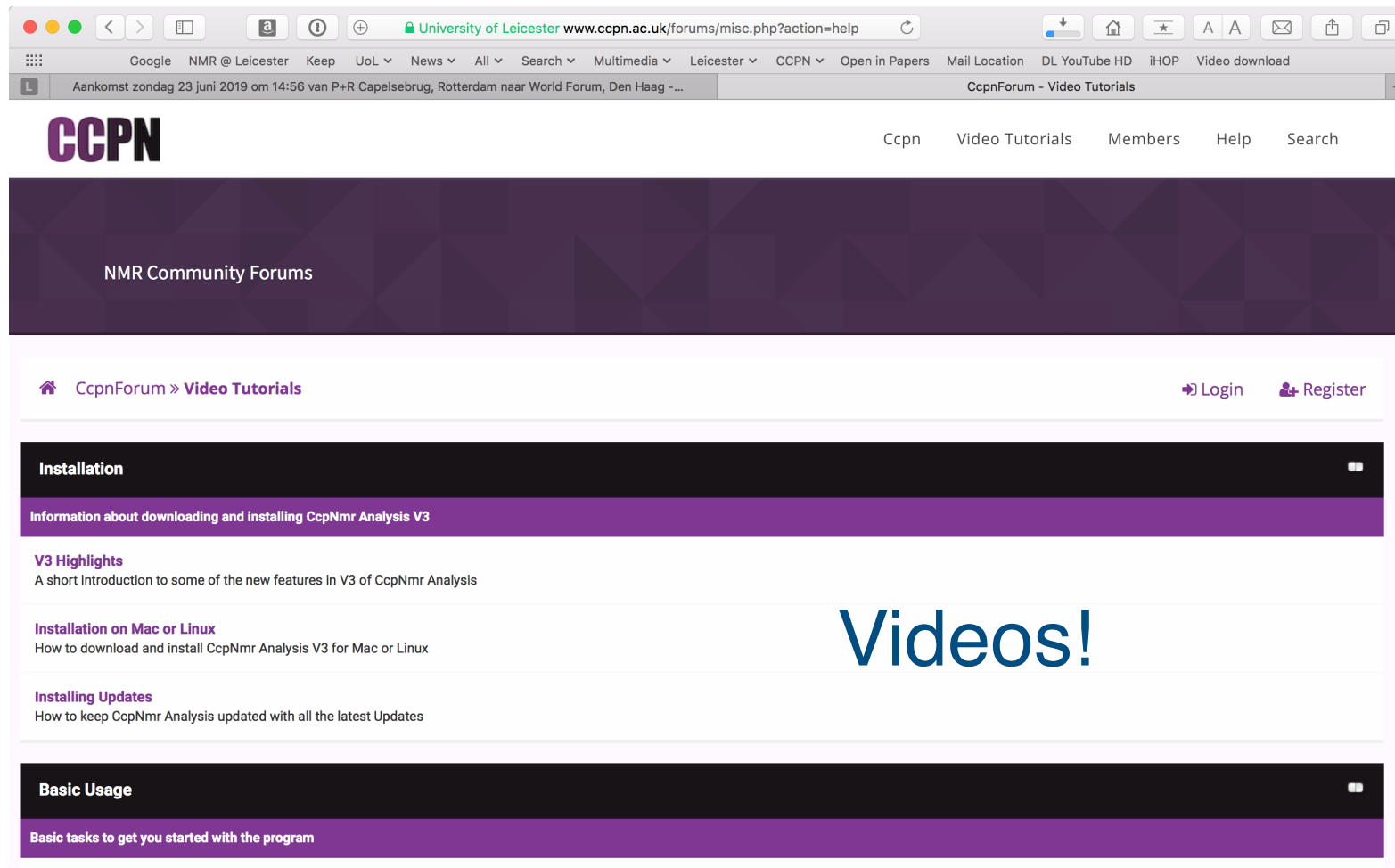
The screenshot shows a web browser window displaying the CcpNmr forum page. The browser's address bar shows the URL www.ccpn.ac.uk/forums/misc.php?action=help. The page features a navigation bar with links to Ccpn, Video Tutorials, Members, Help, and Search. Below the navigation bar, there is a section titled "Metabolomics" with a sub-header "Using Analysis V3 for Metabolomics". A list of video tutorials is displayed, each with a title and a brief description:

- Getting Started: Importing Spectra**
How to import Bruker format spectra
- Creating Stacked Plots**
How to create stacked plots of multiple 1D spectra
- Renaming Spectra**
How to rename a single spectrum or multiple spectra in one go
- Printing to PDF**
How to customise your spectrum display and print to PDF
- Pipeline Processing**
How to create a pipeline to process several 1D spectra at once
- Principal Component Analysis (PCA)**
How to conduct a Principal Component Analysis (PCA) Decomposition
- Overlaying Reference Spectra**
How to overlay experimental with reference spectra
- Picking Peaks**
How to pick peaks
- Annotating Peaks**

Videos!

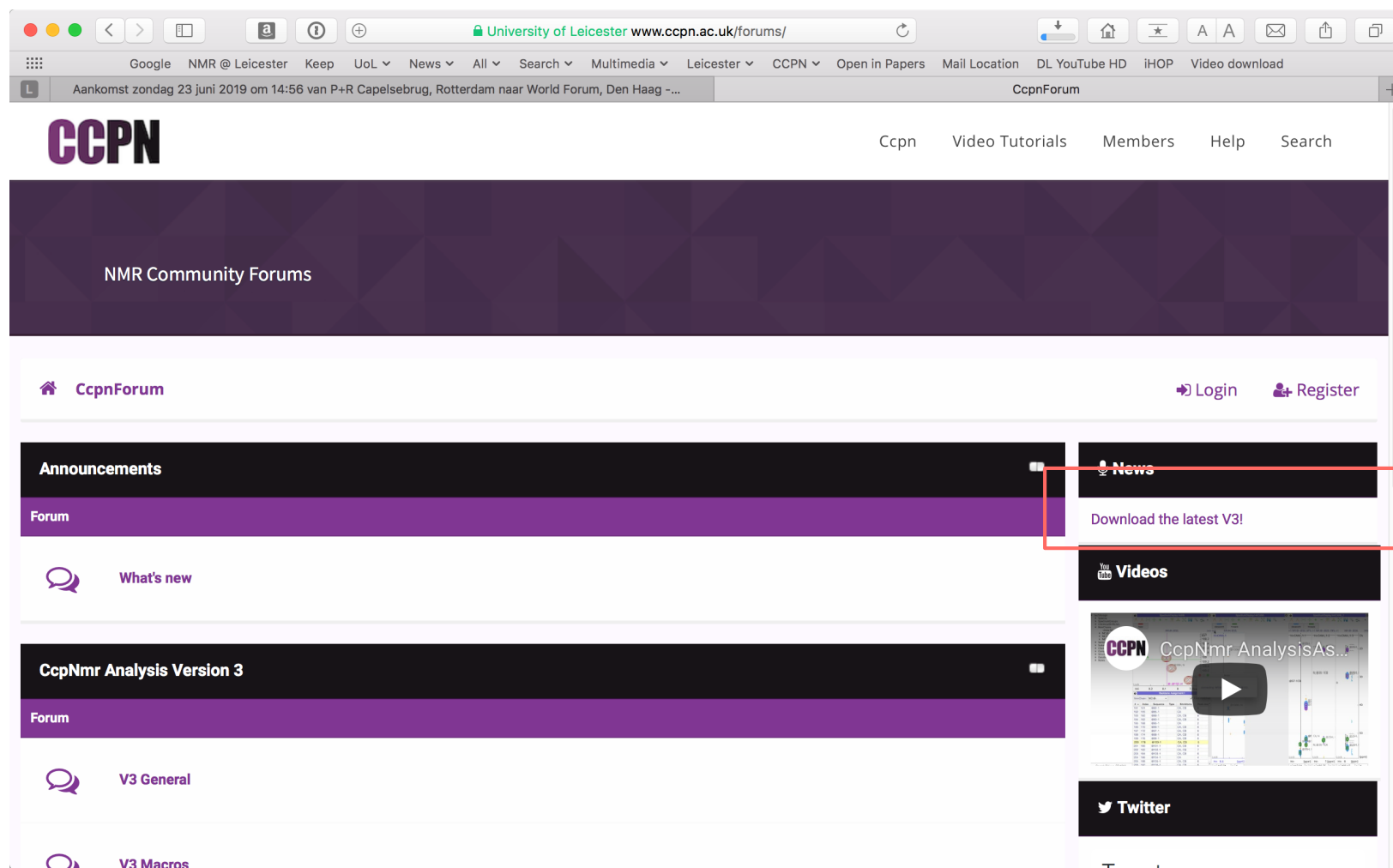
www.ccpn.ac.uk/forums

CcpNmr forum



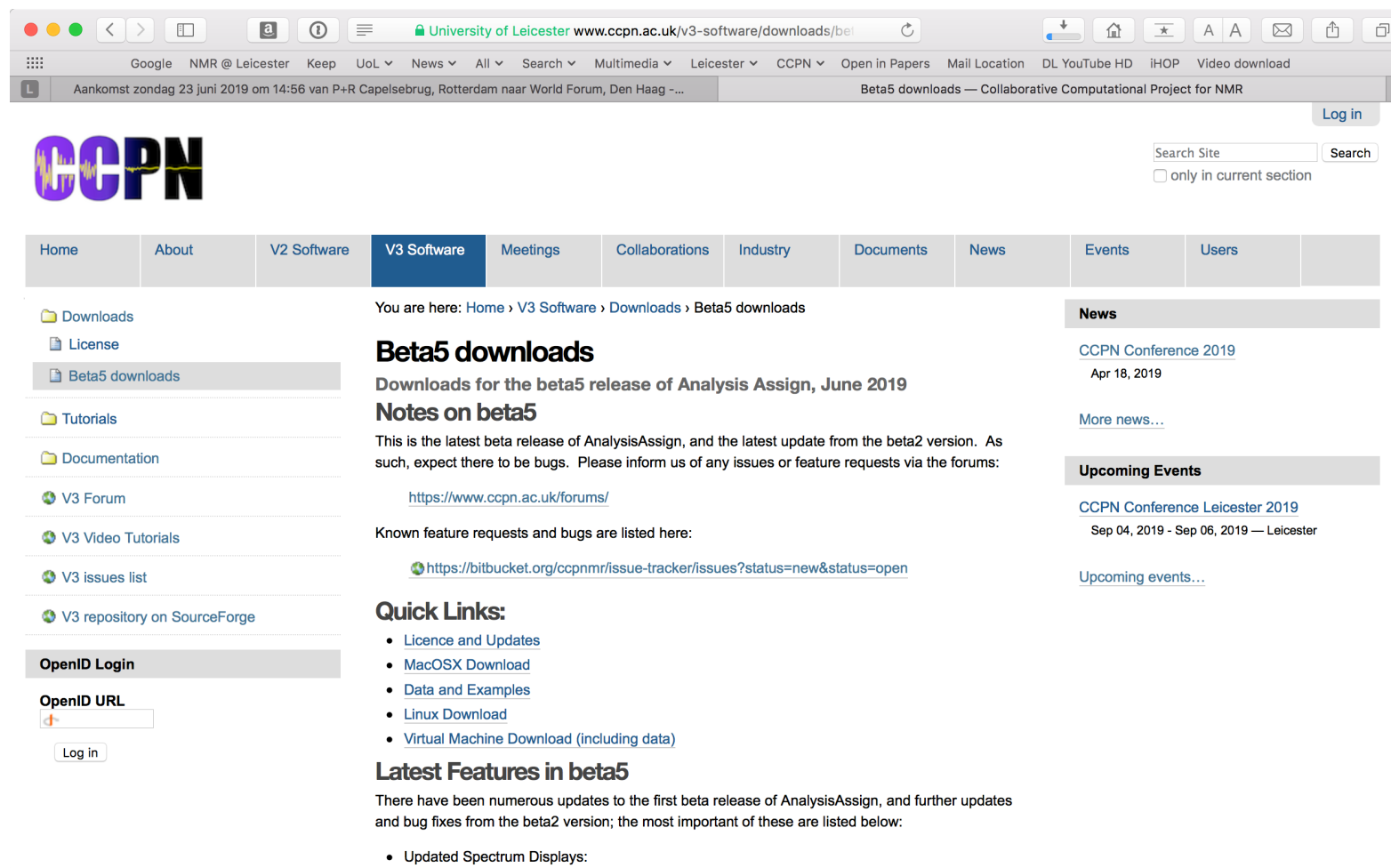
www.ccpn.ac.uk/forums

CcpNmr forum: installation



www.ccpn.ac.uk/forums

CcpNmr forum: installation



The screenshot shows a web browser window displaying the CCPN website. The address bar shows the URL www.ccpn.ac.uk/v3-software/downloads/beta5. The page title is "Beta5 downloads — Collaborative Computational Project for NMR". The CCPN logo is in the top left. A navigation menu includes Home, About, V2 Software, V3 Software (selected), Meetings, Collaborations, Industry, Documents, News, Events, and Users. A left sidebar contains links for Downloads, License, Beta5 downloads (selected), Tutorials, Documentation, V3 Forum, V3 Video Tutorials, V3 issues list, and V3 repository on SourceForge. The main content area is titled "Beta5 downloads" and includes a sub-header "Downloads for the beta5 release of Analysis Assign, June 2019". It contains "Notes on beta5" stating it is the latest beta release, a link to the forums, and a list of "Quick Links" including Licence and Updates, MacOSX Download, Data and Examples, Linux Download, and Virtual Machine Download. A "Latest Features in beta5" section mentions updated spectrum displays. The right sidebar shows "News" with a link to the CCPN Conference 2019 and "Upcoming Events" with a link to the CCPN Conference Leicester 2019.

Bootable Linux
OSX install (USB)
Linux install (USB)

CcpNmr forum: installation

OSX installation issues

