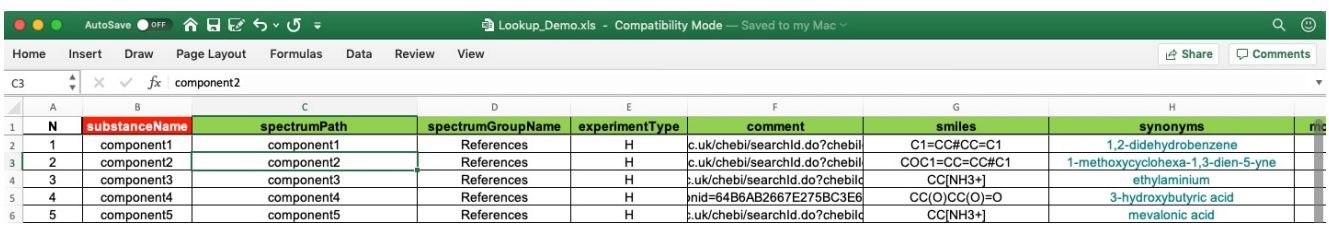
CCPN

CcpNmr AnalysisScreen Version 3

How To's:

Import Data from Excel Lookup File



	A	B	C	D	E	F	G	H
1	N	substanceName	spectrumPath	spectrumGroupName	experimentType	comment	smiles	synonyms
2	1	component1	component1	References	H	c.uk/chebi/searchId.do?chebil	C1=CC#CC=C1	1,2-didehydrobenzene
3	2	component2	component2	References	H	c.uk/chebi/searchId.do?chebil	COC1=CC=CC#C1	1-methoxycyclohexa-1,3-dien-5-yne
4	3	component3	component3	References	H	.uk/chebi/searchId.do?chebilc	CC[NH3+]	ethylaminium
5	4	component4	component4	References	H	nid=64B6AB2667E275BC3E6	CC(O)CC(O)=O	3-hydroxybutyric acid
6	5	component5	component5	References	H	.uk/chebi/searchId.do?chebilc	CC[NH3+]	mevalonic acid

Introduction

In this How To's you will learn how to create an Excel file to load all your spectra and metadata into the program automatically.

Using a lookup file you can easily create CcpNmr objects which, once loaded, will be immediately available in the sidebar.

You will need to use the data located in the **/data/ScreenTutorial** directory of the CCPN V3 examples data which you can download from https://www.ccpn.ac.uk/v3-software/tutorials/tutorial-data-and-examples.

Please note that the images shown are only representative and you may encounter minor differences in your setup.

Start CcpNmr Analysis V3

- Apple users by running Assign/Screen on the Launcher
- Unix users by using the terminal command: *bin/assign* or *screen*
- Windows users by double-clicking on the .*bat* file

1 Import Data from Excel Lookup File

The program can read .xls or .xlxs files with multiple sheets that include the words **Sample** or **Substance** in the sheet name.

You can create files that contain either the Substance or Sample page or both.

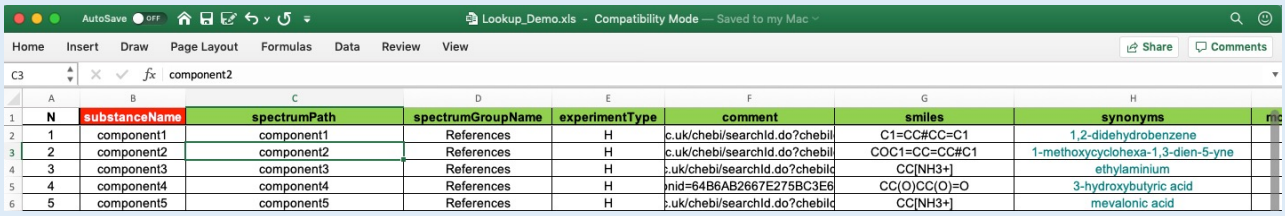
1A Overview

Open a new Excel file or find a template in:
ScreenTutorial/LookupTemplate.xls

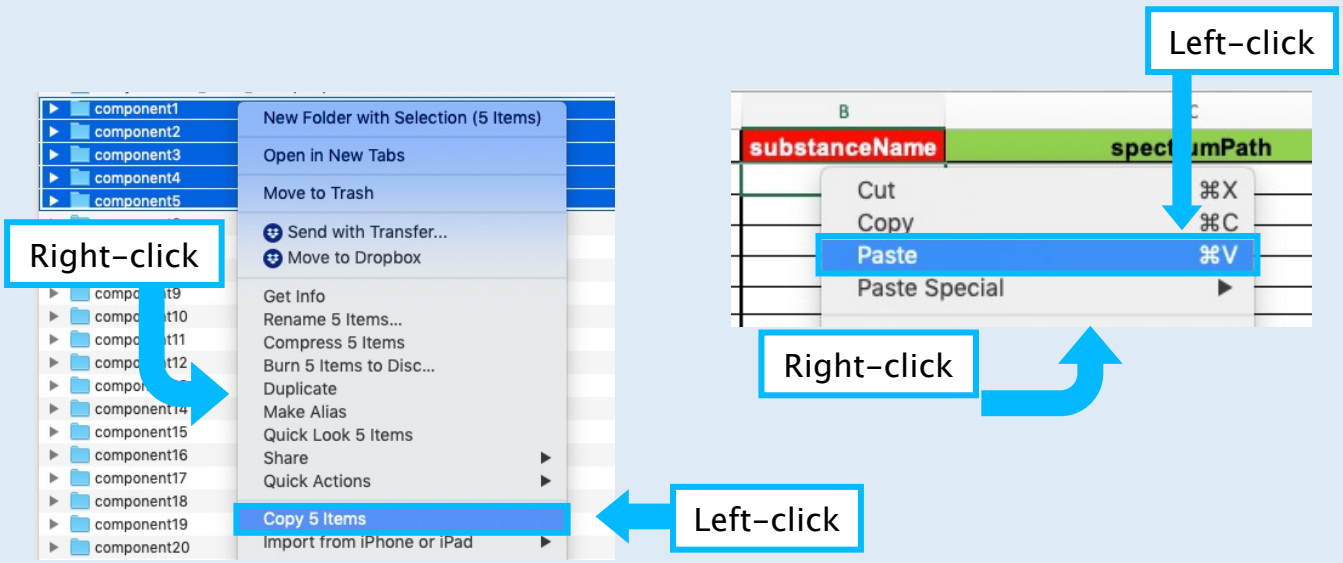
Mandatory Sheet names:
Title must start with “Substance” or “Sample”

Mandatory columns:
Substance sheet:
SubstanceName
Sample sheet:
SampleName

1 Import Data from Excel Lookup File



N	substanceName	spectrumPath	spectrumGroupName	experimentType	comment	smiles	synonyms
1	component1	component1	References	H	c.uk/chebi/searchId.do?chebil	C1=CC#CC=C1	1,2-didehydrobenzene
2	component2	component2	References	H	c.uk/chebi/searchId.do?chebil	COC1=CC=CC#C1	1-methoxycyclohexa-1,3-dien-5-yne
3	component3	component3	References	H	.uk/chebi/searchId.do?chebilc	CC[NH3+]	ethylaminium
4	component4	component4	References	H	nid=64B6AB2667E275BC3E6	CC(O)CC(O)=O	3-hydroxybutyric acid
5	component5	component5	References	H	.uk/chebi/searchId.do?chebilc	CC[NH3+]	mevalonic acid



1B Create the Substance Sheet

The first sheet, **Substance**, can contain metadata associated with small molecules, for example, whose spectra have been used as references in a screen.

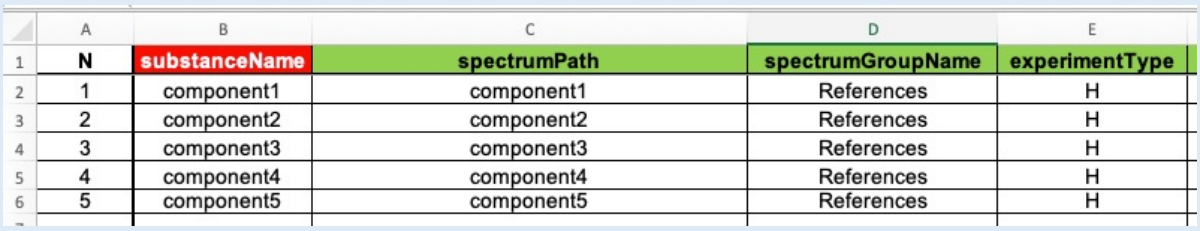
- **Place** the Lookup file template from the **ScreenTutorial** directory to the directory containing your spectra (**ScreenTutorial/spectra/LookupData** if using the tutorial data).
- Open the template and fill in the **substanceName** column. This is the only mandatory column to fill in. A quick way to fill the table on a Mac is to multi-select the directory or spectra files you want to include, then **copy and paste** them into the Excel cell under **substanceName**. Select the first five components.

  OR

  copy and paste the following:

  component1
  component2
  component3
  component4
  component5

1 Import Data from Excel Lookup File



	A	B	C	D	E
1	N	substanceName	spectrumPath	spectrumGroupName	experimentType
2	1	component1	component1	References	H
3	2	component2	component2	References	H
4	3	component3	component3	References	H
5	4	component4	component4	References	H
6	5	component5	component5	References	H

1c Add reference spectrum information

To include the Substance reference spectra, you need to insert the **spectrumPath** (AnalayisScreen will recognise any spectrum format).

You have three options:

1. If all the spectra files are located in the same directory as the lookup file, insert only the file names as above.
2. If the spectra are located in a subdirectory, insert the directory name first followed by a slash and the filename (the relative path starting from the Excel file), e.g. references/component1
3. If the spectra files are located in a completely different location, insert the full path, e.g. /Users/username/Desktop/data3/MySpectra/component1

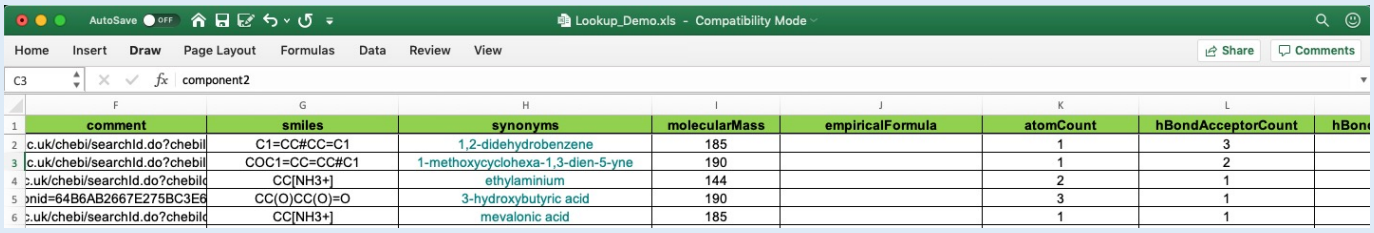
   For Bruker files, you can insert the path to the "r" file: ~ScreenTutorial/spectra/LookupData/component1/pdata/1/1r .

For clarity, we recommend keeping all the files in the same directory together with the Excel lookup file.

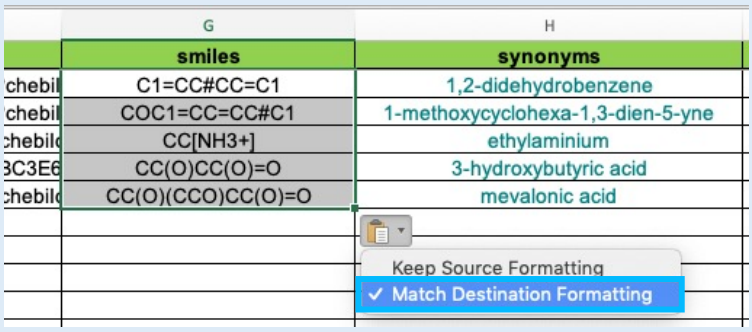
- Insert the **spectrumGroupName**; e.g. References. This will create a **Spectrum Group** with that name and place the spectra into it.

- Insert the **experimentType**. The list of experiment types, their nomenclatures and more information, can be found at https://www.ccpn.ac.uk/v3-software/documentation/v3-experiment-types/view.
  For these 1-dimensional spectra, simply type **H** into the cell.

1 Import Data from Excel Lookup File



	F	G	H	I	J	K	L
1	comment	smiles	synonyms	molecularMass	empiricalFormula	atomCount	hBondAcceptorCount
2	c.uk/chebi/searchId.do?chebil	C1=CC#CC=C1	1,2-didehydrobenzene	185		1	3
3	c.uk/chebi/searchId.do?chebil	COC1=CC=CC#C1	1-methoxycyclohexa-1,3-dien-5-yne	190		1	2
4	.uk/chebi/searchId.do?chebil	CC[NH3+]	ethylaminium	144		2	1
5	nid=64B6AB2667E275BC3E6	CC(O)CC(O)=O	3-hydroxybutyric acid	190		3	1
6	.uk/chebi/searchId.do?chebil	CC[NH3+]	mevalonic acid	185		1	1



1D Add Substance metadata

- The **comment** column will store any textual information about the substance.
- If you enter the **smiles** for your substances, the programme will automatically generate the structures inside the software. For the tutorial, copy and paste these SMILES:

  C1=CC#CC=C1

  COC1=CC=CC#C1

  CC[NH3+]

  CC(O)CC(O)=O

  CC(O)(CCO)CC(O)=O

  In Excel, click on the small folder on the bottom right of the pasted items and select **Match Destination formatting**
- In the **synonyms** column insert the chemical name of the substance and again select **Match Destination formatting**, e.g.

  1,2-didehydrobenzene

  1-methoxycyclohexa-1,3-dien-5-yne

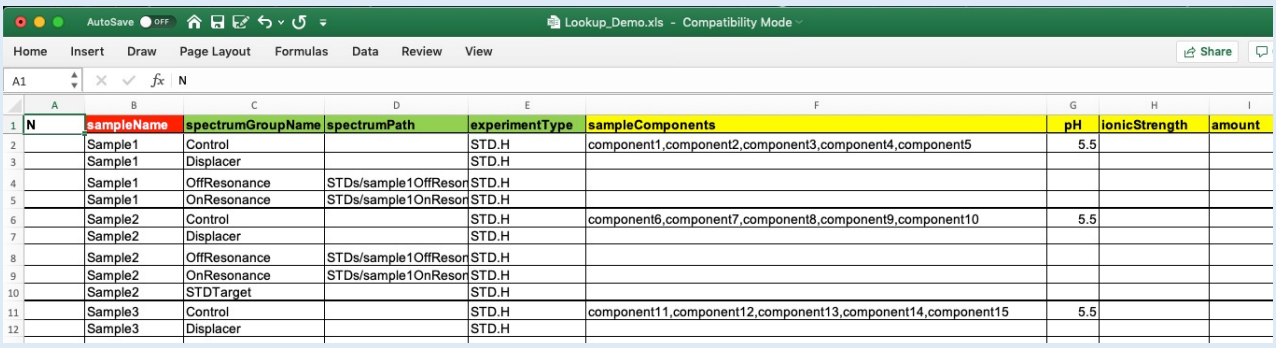
  ethylaminium

  3-hydroxybutyric acid

  mevalonic acid
- All the following columns contain the substance chemical properties. Fill them if you want to display them within the software.
- **Save** the file.

A fully completed lookup is provided at ScreenTutorial/spectra/LookupData/LookupExample.xls. This file can be opened in AnalysisScreen by **dragging and dropping** it into the sidebar or drop area.

1 Import Data from Excel Lookup File



N	sampleName	spectrumGroupName	spectrumPath	experimentType	sampleComponents	pH	ionicStrength	amount
	Sample1	Control		STD.H	component1,component2,component3,component4,component5	5.5		
	Sample1	Displacer		STD.H				
	Sample1	OffResonance	STDs/sample1OffReson	STD.H				
	Sample1	OnResonance	STDs/sample1OnReson	STD.H				
	Sample2	Control		STD.H	component6,component7,component8,component9,component10	5.5		
	Sample2	Displacer		STD.H				
	Sample2	OffResonance	STDs/sample1OffReson	STD.H				
	Sample2	OnResonance	STDs/sample1OnReson	STD.H				
	Sample2	STDTarget		STD.H				
	Sample3	Control		STD.H	component11,component12,component13,component14,component15	5.5		
	Sample3	Displacer		STD.H				

1E Create the Samples Sheet

The next sheet in the template is **Samples**. This can contain metadata associated with particular samples, e.g. in a screening trial the sample could contain lots of spectra recorded with different experimental conditions. The only mandatory column is the **sampleName** column.

- Insert the **sampleName** in the first column, e.g. **Sample1**

The next three columns are specific to the spectra recorded for this sample:

- Insert the **spectrumGroupName**, e.g. **STD_Target**, if you want the spectrum to be included in a Spectrum Group
- Insert the **spectrumPath**, e.g. **STDs/Sample1_Std** (see the section 9C for how to insert the spectrum path)
- Insert the spectrum: **experimentType**, e.g. **STD.H** (see the documentation for information on the **Experiment Type** nomenclature)

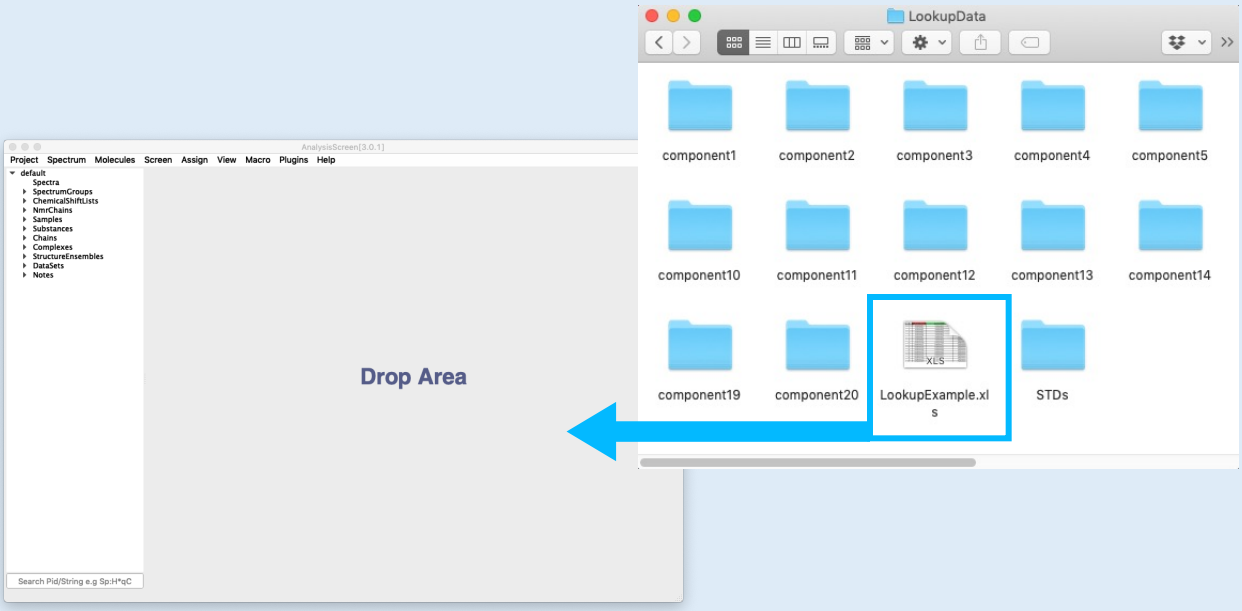
- Fill in the **sampleComponents** column. Insert the names of the components that are present in the sample. In the case of a mixture containing components 1 to 5, insert as a comma-separated list without spaces:

  component1,component2,component3,component4,component5
- The other columns record a sample's chemical properties and other information. Fill them in if you want to display them within the software.

To add extra spectra for the same sample, repeat points 1 to 3 as shown in the figure. There is no need to duplicate the samples properties (yellow columns) as long as the sample name is the same. If you add the same information twice, only the first entry will be considered.

To add an extra sample, simply fill in further rows.

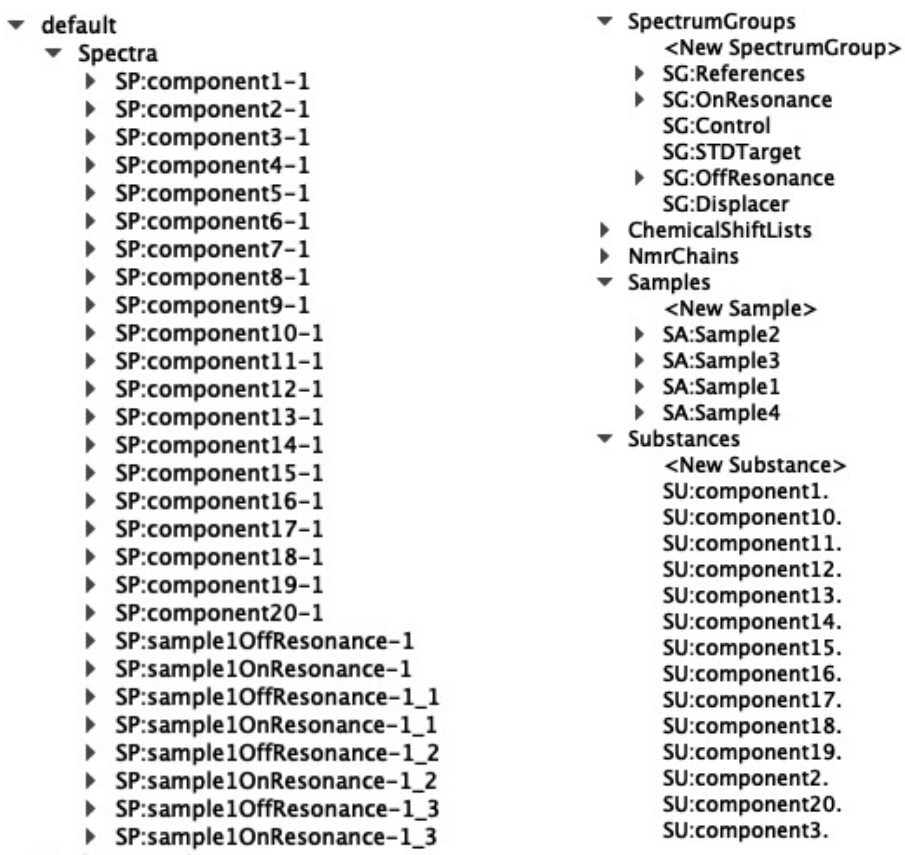
1 Import Data from Excel Lookup File



1F Import Excel Lookup File into AnalysisScreen

- **Drag and Drop** the **LookupExample.xls** file located in the **ScreenTutorial/spectra/LookupData** directory of the tutorial data from your file browser into the **sidebar** or **drop area** of AnalysisScreen.

You will now be able to see all the imported data in the sidebar.



Please note that you cannot drop the same lookup file containing the same values into the same project twice. This is because the project cannot create new objects with pre-existing names. When dropping the same file onto a project twice, only the first entries will be used.

Contact Us

Website:
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Suggestions and comments:
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Issues and bug reports:
https://www.ccpn.ac.uk/forums

Cite Us

Mureddu, L. et al. CcpNmr AnalysisScreen, a new software programme with dedicated automated analysis tools for fragment-based drug discovery by NMR. J. Biomol. NMR (2020)

Skinner, S. P. et al. CcpNmr AnalysisAssign: a flexible platform for integrated NMR analysis. J. Biomol. NMR 66, (2016)