CCPN

CcpNmr AnalysisScreen Version 3

How To

Create a NEF file from tabular data

```
data_project_1

   save_nef_nmr_meta_data

      _nef_nmr_meta_data.sf_category      nef_nmr_meta_data
      _nef_nmr_meta_data.sf_framecode     nef_nmr_meta_data
      _nef_nmr_meta_data.format_name      nmr_exchange_format
      _nef_nmr_meta_data.format_version   1.1
      _nef_nmr_meta_data.program_name     AnalysisAssign
      _nef_nmr_meta_data.program_version  3.1.0
      _nef_nmr_meta_data.creation_date    2022-11-24T01:38:01.267301
      _nef_nmr_meta_data.uuid             AnalysisAssign-2022-11-24T01:38:01.267301-962017545
      _nef_nmr_meta_data.coordinate_file_name  .
   save_


   save_nef_molecular_system

      _nef_molecular_system.sf_category   nef_molecular_system
      _nef_molecular_system.sf_framecode  nef_molecular_system

      loop_
         _nef_sequence.index
         _nef_sequence.chain_code
         _nef_sequence.sequence_code
         _nef_sequence.residue_name
         _nef_sequence.linking
         _nef_sequence.residue_variant
         _nef_sequence.cis_peptide

         1   A  3   ASN  start   .                .
         2   A  4   MET  middle  .                .
         3   A  5   LYS  middle  .                .
         4   A  6   LEU  middle  .                .
         5   A  57   GLY  middle  .                .
         6   A  58   GLN  middle  .                .
      stop_
   save_


   save_nef_chemical_shift_list_default

      _nef_chemical_shift_list.sf_category   nef_chemical_shift_list
      _nef_chemical_shift_list.sf_framecode  nef_chemical_shift_list_default

      loop_
         _nef_chemical_shift.chain_code
         _nef_chemical_shift.sequence_code
         _nef_chemical_shift.residue_name
         _nef_chemical_shift.atom_name
         _nef_chemical_shift.value
         _nef_chemical_shift.value_uncertainty
         _nef_chemical_shift.element
         _nef_chemical_shift.isotope_number

         A  3   ASN  H     8.142210567  .            H  1
         A  3   ASN  N     114.2228732  .            N  15
         A  4   MET  H     8.474162011  .            H  1
         A  4   MET  N     120.4901187  .            N  15
         A  5   LYS  H     8.34699653   .            H  1
         A  5   LYS  N     121.4128882  .            N  15
         A  6   LEU  H     8.487866533  .            H  1
         A  6   LEU  N     124.721835   .            N  15
         A  7   GLY  H     8.288431248  .            H  1
      stop_
   save_
```

Introduction

This *How To* will show you how to create a NEF file from tabular data for import into CcpNmr Analysis Version 3.1.
We would like to emphasise that **this is NOT really something we recommend doing** and it is certainly not what the NMR Exchange Format (NEF) was created for. However, we do realise that this may the be only way to deal with certain types of data (in particular old legacy data) unless you want to get into some scripting. And this is certainly something useful that members of CCPN team have been known to do from time to time and we felt it was worth sharing.

You will need to use the data located in the **HowTo_CreateNEFFromTabularData** directory of the CcpNmr V3 NEF exmple data which you can download from the CCPN website https://ccpn.ac.uk/support/tutorials/.

It is assumed that you have some basic familiarity with the program, e.g. from having completed our Beginners Tutorial.
Please note that the images shown are only representative and you may encounter minor differences to your setup.

Start CcpNmr Analysis V3

Apple and Linux users by using the terminal command: *bin/assign*

Windows users by double-clicking on the *assign.bat* file

NMRbox users by using the terminal command *analysisassign*

Introduction

NEF Files

The template.nef file which we have supplied is split into four parts:

save_nef_nmr_meta_data – general information about the file *(mandatory)*

save_nef_molecular_system – sequence information *(mandatory)*

save_nef_chemical_shift_list – chemical shift list *(mandatory)*

save_nef_nmr_spectrum – spectrum information and peak list *(optional)*

Each of these has a minimal set of information which has to be included in order that the file will be recognised as a NEF file.

For more information on NEF files and their specification, please visit https://www.ccpn.ac.uk/manual/v3/NEF.html

```
data_default
```

This first line always has be included. You can replace the word **default** by something else related to your data if you wish.

```
save_nef_nmr_meta_data

    _nef_nmr_meta_data.sf_category      nef_nmr_meta_data
    _nef_nmr_meta_data.sf_framecode     nef_nmr_meta_data
    _nef_nmr_meta_data.format_name      nmr_exchange_format
    _nef_nmr_meta_data.format_version   1.1
    _nef_nmr_meta_data.program_name     myNEFmaker
    _nef_nmr_meta_data.program_version  0.1
    _nef_nmr_meta_data.creation_date    2022-02-11
    _nef_nmr_meta_data.uuid             NEFmaker0001-00000001

save_
```

In principle, **_nef_nmr_meta_data.creation_date** and **_nef_nmr_meta_data.uuid** should be unique for each NEF file, but for this usage you can just leave them as they are (or change/adjust it if you would like).

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```
save_nef_molecular_system

  _nef_molecular_system.sf_category   nef_molecular_system
  _nef_molecular_system.sf_framecode  nef_molecular_system

  loop_
     _nef_sequence.index
     _nef_sequence.chain_code
     _nef_sequence.residue_name
     _nef_sequence.sequence_code

1       A       ALA     1
2       A       LEU     2
3       A       ALA     3

stop_
save_
```

The **save_nef_molecular_system** part contains a table with 4 mandatory columns:

index, **chain_code**, **residue_name**, **sequence_code**

The order of these columns is not important as long as their order corresponds to the order of the "column headers" specified following the word **loop_**.

The **index** is simply a list of consecutive numbers (essentially the row number).

The **sequence_codes** do not have to consecutive and can even be negative (e.g. if they refer to a tag).

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```
save_nef_chemical_shift_list_shifts

   _nef_chemical_shift_list.sf_category   nef_chemical_shift_list
   _nef_chemical_shift_list.sf_framecode  nef_chemical_shift_list_shifts


   loop_
      _nef_chemical_shift.chain_code
      _nef_chemical_shift.value
      _nef_chemical_shift.value_uncertainty
      _nef_chemical_shift.sequence_code
      _nef_chemical_shift.residue_name
      _nef_chemical_shift.atom_name

A       129.447 0.1     1       ALA     N
A       7.475   0.001   1       ALA     H
A       56.398  0.1     2       LEU     CA
A       176.674 0.1     2       LEU     C
A       8.435   0.001   3       ALA     H
A       122.58  0.1     3       ALA     N

stop_
save_
```

The **save_nef_chemical_shift_list_shifts** part contains a table with 5 mandatory columns:

chain_code, sequence_code, residue_name, atom_name, (chemical shift) **value**

The order of these columns is not important as long as their order corresponds to the order of the "column headers" specified following the word **loop_**.

The **atom_name** is arbitrary and does not have to follow the NEF atom naming convention.

The (chemical shift) **value_uncertainty** is optional.

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```
save_nef_nmr_spectrum_anyName

   _nef_nmr_spectrum.sf_category                 nef_nmr_spectrum
   _nef_nmr_spectrum.sf_framecode                nef_nmr_spectrum_anyName
   _nef_nmr_spectrum.num_dimensions              2
   _nef_nmr_spectrum.chemical_shift_list         nef_chemical_shift_list_shifts

    loop_
       _nef_spectrum_dimension.dimension_id
       _nef_spectrum_dimension.axis_unit
       _nef_spectrum_dimension.axis_code

       1  ppm  1H
       2  ppm  15N
    stop_

    loop_
       _nef_spectrum_dimension_transfer.dimension_1
       _nef_spectrum_dimension_transfer.dimension_2
       _nef_spectrum_dimension_transfer.transfer_type
       _nef_spectrum_dimension_transfer.is_indirect

       1  2  onebond  false
    stop_

    loop_
       _nef_peak.index
       _nef_peak.peak_id
       _nef_peak.volume
       _nef_peak.volume_uncertainty
       _nef_peak.height
       _nef_peak.height_uncertainty
       _nef_peak.position_1
       _nef_peak.position_uncertainty_1
       _nef_peak.position_2
       _nef_peak.position_uncertainty_2
       _nef_peak.chain_code_1
       _nef_peak.sequence_code_1
       _nef_peak.residue_name_1
       _nef_peak.atom_name_1
       _nef_peak.chain_code_2
       _nef_peak.sequence_code_2
       _nef_peak.residue_name_2
       _nef_peak.atom_name_2

       1   1    .  .  791958.375   .  8.458275971  .  122.2694881  .  A  3  ALA   H  A  3  ALA   N
       2   2    .  .  946877.625   .  8.930837073  .  129.3918342  .  .  .  .   .    .  .  .   .    .

stop_
save_
```

We won't be using the **save_nef_molecular_system** part in this **How To**, but you may wish to use it for your own purposes.

Mandatory sections are highlighted. Note that none of the peak table columns are mandatory!

1 Creating a NEF file from tabular data

Our task is to create a NEF file containig the data contained in the **protein.seq** and **shifts.txt** files of the example data, so that this can be imported into CcpNmr Analysis.

We will use the **template.nef** file as our template to build our final NEF file. We will do this by creating tables in Excel or another spreadsheet program which we will then copy into the template.nef file.

The **shifts.nef** file is an example of the complete NEF file. The **template_shifts.xlsx** file is an example Excel file with template and example sheets.

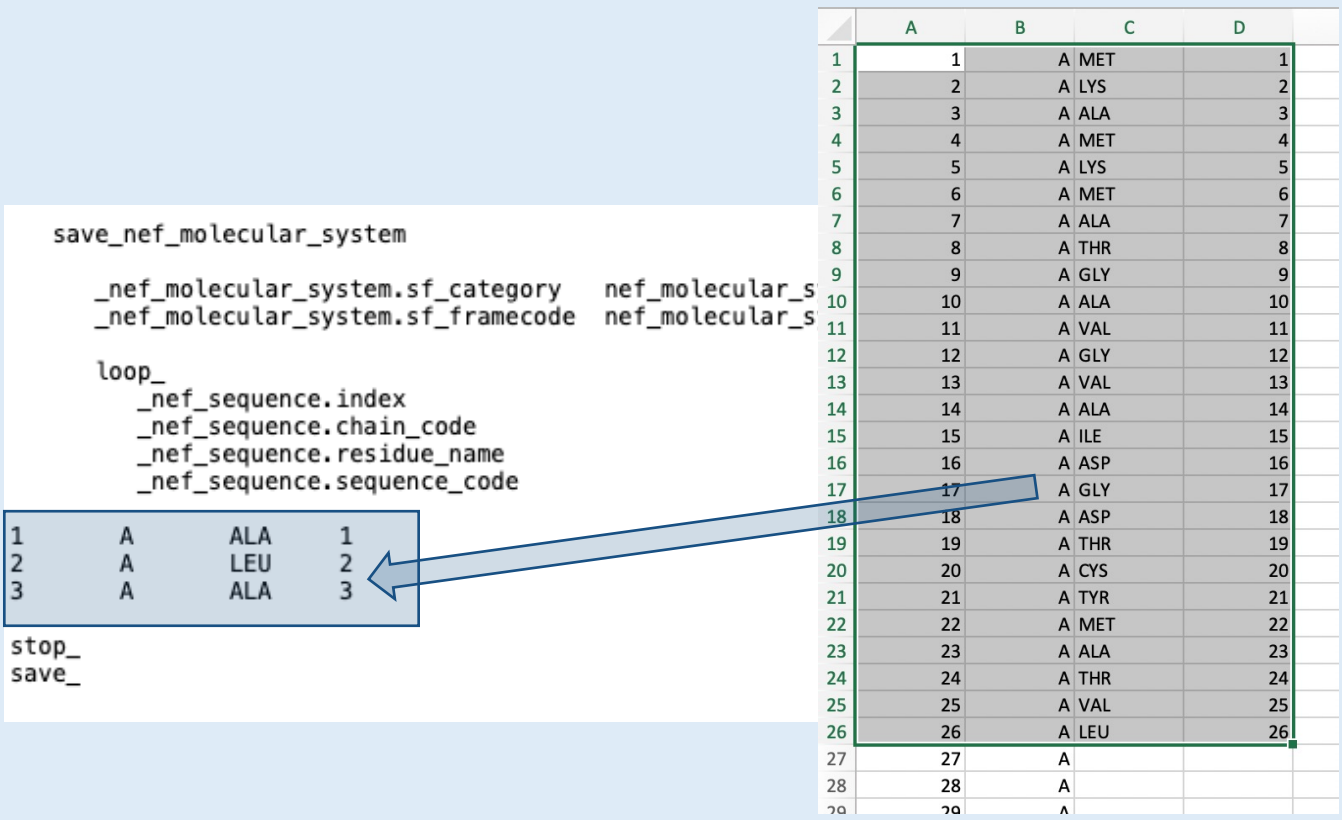
```
save_nef_nmr_meta_data

   _nef_nmr_meta_data.sf_category       nef_nmr_meta_data
   _nef_nmr_meta_data.sf_framecode      nef_nmr_meta_data
   _nef_nmr_meta_data.format_name       nmr_exchange_format
   _nef_nmr_meta_data.format_version    1.1
   _nef_nmr_meta_data.program_name      myNEFmaker
   _nef_nmr_meta_data.program_version   0.1
   _nef_nmr_meta_data.creation_date     2022-02-11
   _nef_nmr_meta_data.uuid              NEFmaker0001-00000001

save_
```

1A Creating the Meta Data section

Simply retain this secton as-is.

If you like, you can change the **nef_nmr_meta_data.creation_date** and **_nef_nmr_meta_data.uuid** entries, as these should technically be different for every NEF file. But the purposes here this doesn't really matter.

1 Creating a NEF file from tabular data



	A	B	C	D
1	1	A	MET	1
2	2	A	LYS	2
3	3	A	ALA	3
4	4	A	MET	4
5	5	A	LYS	5
6	6	A	MET	6
7	7	A	ALA	7
8	8	A	THR	8
9	9	A	GLY	9
10	10	A	ALA	10
11	11	A	VAL	11
12	12	A	GLY	12
13	13	A	VAL	13
14	14	A	ALA	14
15	15	A	ILE	15
16	16	A	ASP	16
17	17	A	GLY	17
18	18	A	ASP	18
19	19	A	THR	19
20	20	A	CYS	20
21	21	A	TYR	21
22	22	A	MET	22
23	23	A	ALA	23
24	24	A	THR	24
25	25	A	VAL	25
26	26	A	LEU	26
27	27	A		
28	28	A		

1B Creating the Molecular System section

Retain everything apart from the actual table.

We will recreate the table in Excel (or other spreadsheet software) and then copy it into that position.

The first two columns (**_nef_sequence.index** and **_nef_sequence.chain_code**) can be prepared easily in Excel: the index is just a consecutive number and the chain code is usually a capital letter, e.g. **A**.

An example is provide in the **template** sheet of the **template_shifts.xlsx** file.

You can copy the **_nef_sequence.residue_name** column from the **protein.seq file** provided**.**

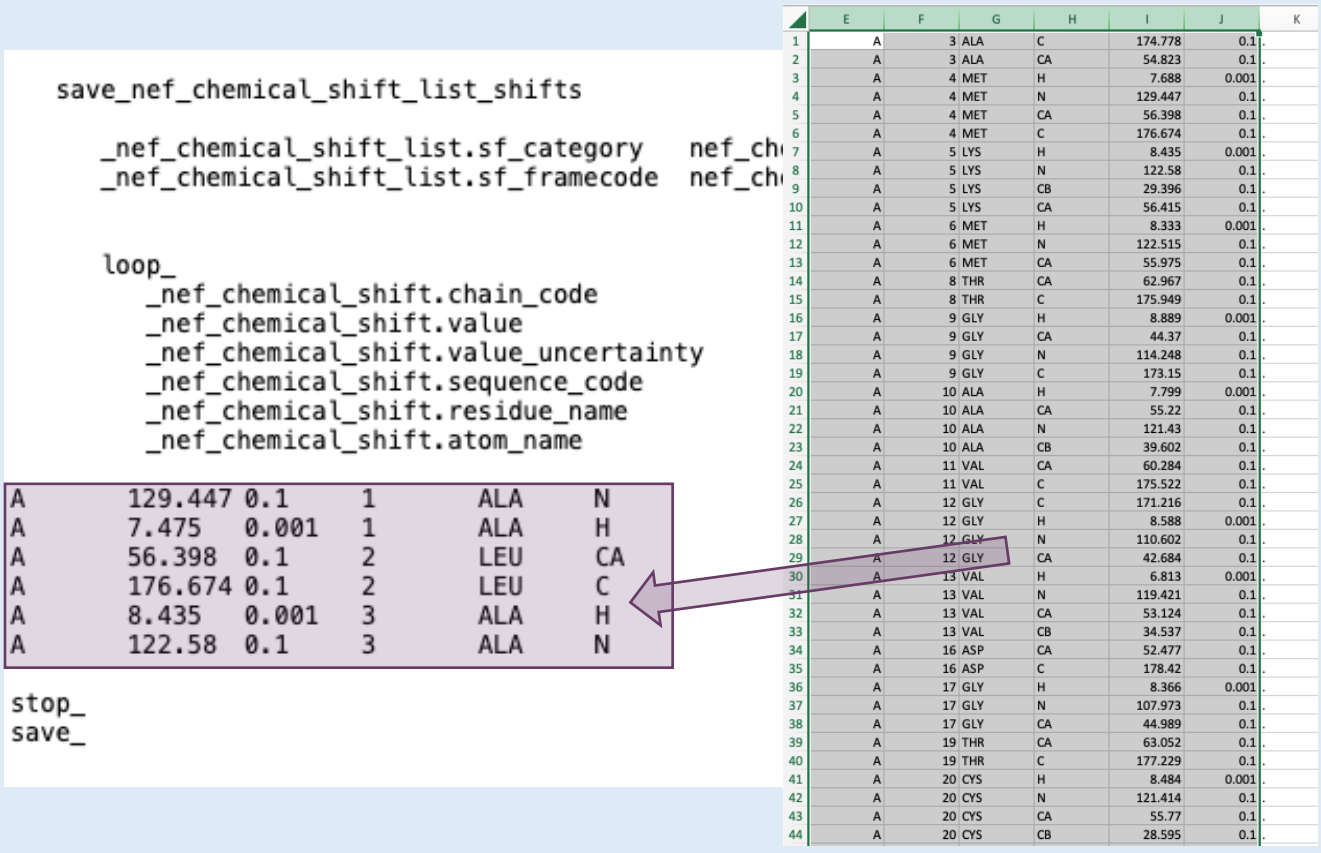
Then add another column with consecutive numbers for the **_nef_sequence.sequence_code**.

An example is provide in the **sequence** sheet of the **template_shifts.xlsx** file.

Now copy the first four columns of your spreadsheet and paste them into the **template.nef** as shown above.

1 Creating a NEF file from tabular data

```
save_nef_chemical_shift_list_shifts

    _nef_chemical_shift_list.sf_category    nef_ch
    _nef_chemical_shift_list.sf_framecode   nef_ch


    loop_
       _nef_chemical_shift.chain_code
       _nef_chemical_shift.value
       _nef_chemical_shift.value_uncertainty
       _nef_chemical_shift.sequence_code
       _nef_chemical_shift.residue_name
       _nef_chemical_shift.atom_name

A       129.447 0.1     1       ALA     N
A       7.475   0.001   1       ALA     H
A       56.398  0.1     2       LEU     CA
A       176.674 0.1     2       LEU     C
A       8.435   0.001   3       ALA     H
A       122.58  0.1     3       ALA     N

stop_
save_
```

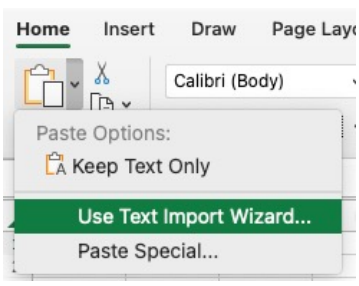


	E	F	G	H	I	J	K
1	A	3	ALA	C	174.778	0.1	
2	A	3	ALA	CA	54.823	0.1	
3	A	4	MET	H	7.688	0.001	
4	A	4	MET	N	129.447	0.1	
5	A	4	MET	CA	56.398	0.1	
6	A	4	MET	C	176.674	0.1	
7	A	5	LYS	H	8.435	0.001	
8	A	5	LYS	N	122.58	0.1	
9	A	5	LYS	CB	29.396	0.1	
10	A	5	LYS	CA	56.415	0.1	
11	A	6	MET	H	8.333	0.001	
12	A	6	MET	N	122.515	0.1	
13	A	6	MET	CA	55.975	0.1	
14	A	8	THR	CA	62.967	0.1	
15	A	8	THR	C	175.949	0.1	
16	A	9	GLY	H	8.889	0.001	
17	A	9	GLY	CA	44.37	0.1	
18	A	9	GLY	N	114.248	0.1	
19	A	9	GLY	C	173.15	0.1	
20	A	10	ALA	H	7.799	0.001	
21	A	10	ALA	CA	55.22	0.1	
22	A	10	ALA	N	121.43	0.1	
23	A	10	ALA	CB	39.602	0.1	
24	A	11	VAL	CA	60.284	0.1	
25	A	11	VAL	C	175.522	0.1	
26	A	12	GLY	C	171.216	0.1	
27	A	12	GLY	H	8.588	0.001	
28	A	12	GLY	N	110.602	0.1	
29	A	12	GLY	CA	42.684	0.1	
30	A	13	VAL	H	6.813	0.001	
31	A	13	VAL	N	119.421	0.1	
32	A	13	VAL	CA	53.124	0.1	
33	A	13	VAL	CB	34.537	0.1	
34	A	16	ASP	CA	52.477	0.1	
35	A	16	ASP	C	178.42	0.1	
36	A	17	GLY	H	8.366	0.001	
37	A	17	GLY	N	107.973	0.1	
38	A	17	GLY	CA	44.989	0.1	
39	A	19	THR	CA	63.052	0.1	
40	A	19	THR	C	177.229	0.1	
41	A	20	CYS	H	8.484	0.001	
42	A	20	CYS	N	121.414	0.1	
43	A	20	CYS	CA	55.77	0.1	
44	A	20	CYS	CB	28.595	0.1	

1C Creating the Chemical Shift List section

Select and copy everything from **shifts.txt** and paste into an Excel spreadsheet. We recommend to using the **Text Import Wizard** and splitting the text into columns.

An example is provide in the **raw_data** sheet of the **template_shifts.xlsx** file.



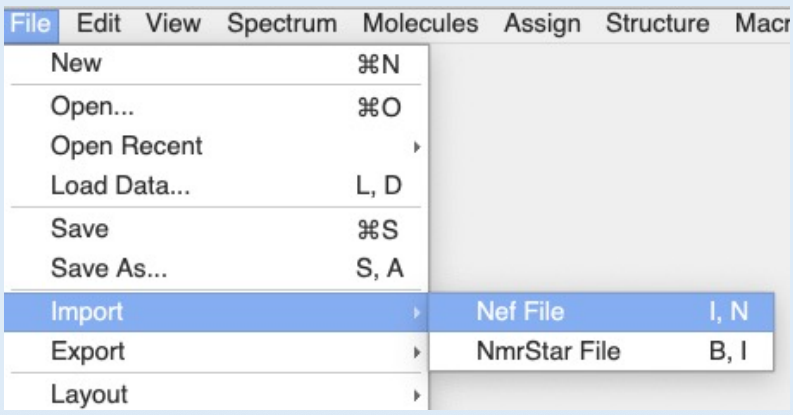
To prepare the table for the **save_nef_chemical_shift_list** section of the NEF file you need to add a column indicating the chain_code (letter **A**) to your data in **column E** (see the **modified_data** sheet 4 in **template_shifts.xlsx**).

Now you can copy **columns E-J** and paste it into the **template.nef** file as shown above.

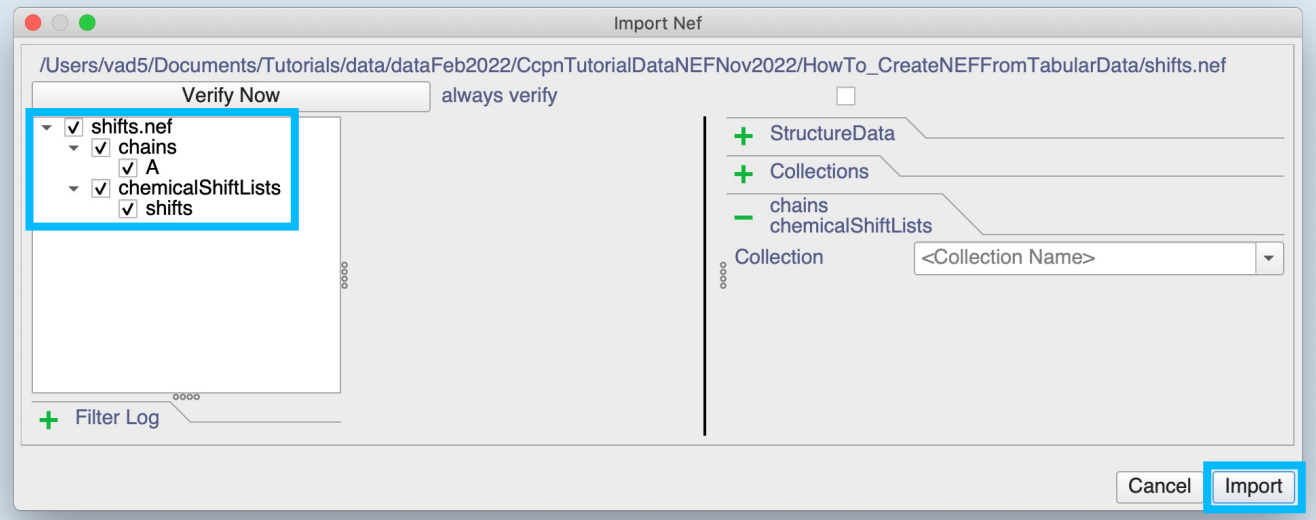
Finally, adjust the order of the tags below the word **loop_** to reflect the order of your data:

```
columns:      new order:

E                       _nef_chemical_shift.chain_code
F                       _nef_chemical_shift.sequence_code
G                       _nef_chemical_shift.residue_name
H                       _nef_chemical_shift.atom_name
I                       _nef_chemical_shift.value
J                       _nef_chemical_shift.value_uncertainty
```

1 Creating a NEF file from tabular data



Shortcut
IN



1D Open the NEF file in CcpNmr Analysis

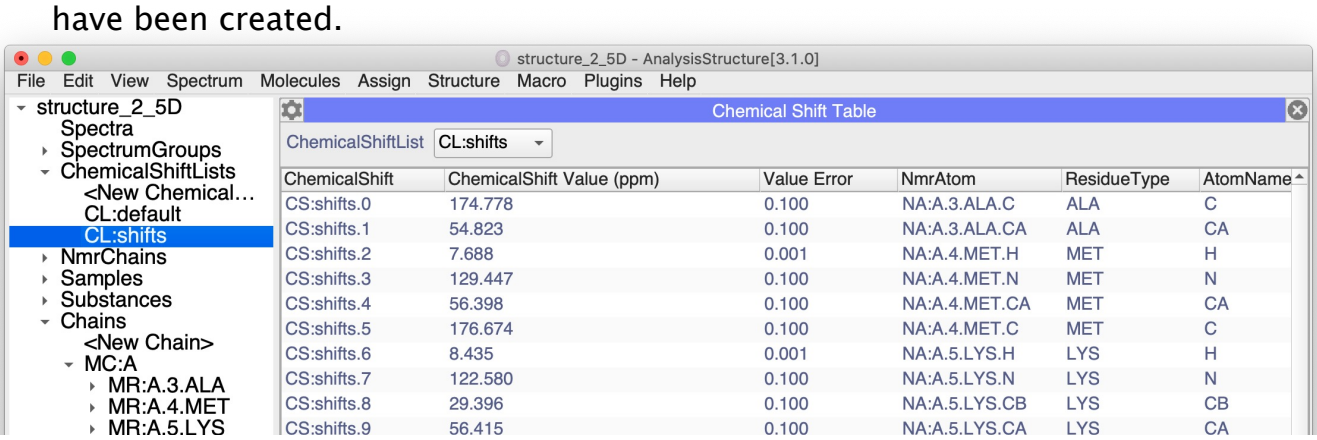
You can check that everything has worked as it should have done by importing your newly created NEF file into CcpNmr Analysis.

Either drag the file from a file browser into the Drop Area or sidebar of the program, or go to **Main Menu → File → Import → Nef File** (or use shortcut **IN**) and select your **.nef** file.

When prompted, choose **Import**.

In the **Import Nef** dialog, tick **shifts.nef** and click on **Import** in order to import both the sequence and chemical shifts.

Now check that the **ChemicalShiftList** and **Chain** have been imported. You will notice that a set of **NmrAtoms** contained within an **NmrChain** will also have been created.



For more details about importing NEF files, see our **How To Import/Export NEF files** available on our website https://ccpn.ac.uk/support/tutorials/.

Contact Us

Website:
www.ccpn.ac.uk

Suggestions and comments:
support@ccpn.ac.uk

Issues and bug reports:
https://forum.ccpn.ac.uk/

Cite Us

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

Cite NEF

Gutmanas, A. et al. NMR Exchange Format: A unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology 22, 433–434 (2015)