

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 be the 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 example 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 to 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).

Introduction

save_nef_molecular_system																			
<table><tr><td>_nef_molecular_system.sf_category</td><td colspan="3">nef_molecular_system</td></tr><tr><td>_nef_molecular_system.sf_framecode</td><td colspan="3">nef_molecular_system</td></tr></table>				_nef_molecular_system.sf_category	nef_molecular_system			_nef_molecular_system.sf_framecode	nef_molecular_system										
_nef_molecular_system.sf_category	nef_molecular_system																		
_nef_molecular_system.sf_framecode	nef_molecular_system																		
loop_																			
<table><tr><td>_nef_sequence.index</td><td colspan="3"></td></tr><tr><td>_nef_sequence.chain_code</td><td colspan="3"></td></tr><tr><td>_nef_sequence.residue_name</td><td colspan="3"></td></tr><tr><td>_nef_sequence.sequence_code</td><td colspan="3"></td></tr></table>				_nef_sequence.index				_nef_sequence.chain_code				_nef_sequence.residue_name				_nef_sequence.sequence_code			
_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 be consecutive and can even be negative (e.g. if they refer to a tag).

Introduction

```
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.

Introduction

```
save_nef_nmr_spectrum_anyName
```

<code>_nef_nmr_spectrum.sf_category</code>	<code>nef_nmr_spectrum</code>
<code>_nef_nmr_spectrum.sf_framecode</code>	<code>nef_nmr_spectrum_anyName</code>
<code>_nef_nmr_spectrum.num_dimensions</code>	<code>2</code>
<code>_nef_nmr_spectrum.chemical_shift_list</code>	<code>nef_chemical_shift_list_shifts</code>

```
loop_
```

<code>_nef_spectrum_dimension.dimension_id</code>
<code>_nef_spectrum_dimension.axis_unit</code>
<code>_nef_spectrum_dimension.axis_code</code>

```
1 ppm 1H
2 ppm 15N
```

```
stop_
```

```
loop_
```

<code>_nef_spectrum_dimension_transfer.dimension_1</code>
<code>_nef_spectrum_dimension_transfer.dimension_2</code>
<code>_nef_spectrum_dimension_transfer.transfer_type</code>
<code>_nef_spectrum_dimension_transfer.is_indirect</code>

```
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 containing 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 section 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

```
save_nef_molecular_system

  _nef_molecular_system.sf_category  nef_molecular_s
  _nef_molecular_system.sf_framecode nef_molecular_s

  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_
```

	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		
29	29	A		

1_B 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

stop_
save_
```

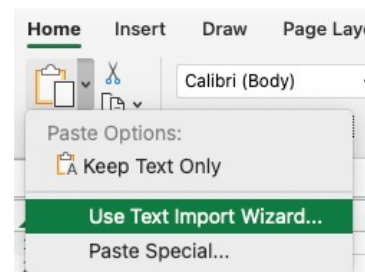
A	129.447	0.1	1	ALA	N
A	7.475	0.001	1	ALA	H
A	56.398	0.1	2	LEU	CA
A	176.674	0.1	2	LEU	C
A	8.435	0.001	3	ALA	H
A	122.58	0.1	3	ALA	N

	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**).

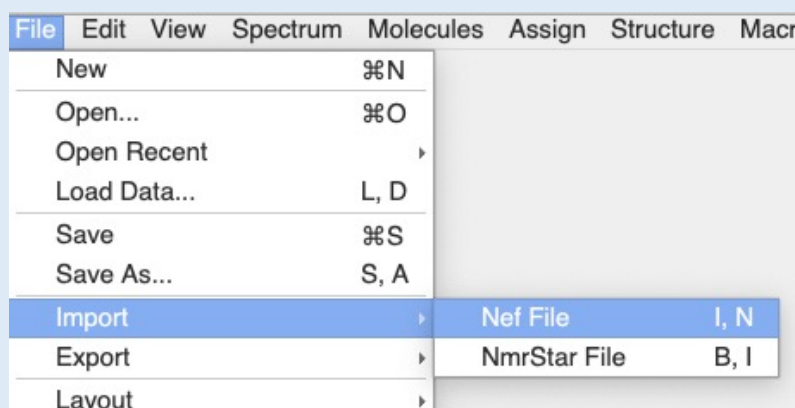
Now you can copy **columns E-J** and paste it into the **template.nef** file as shown above.

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

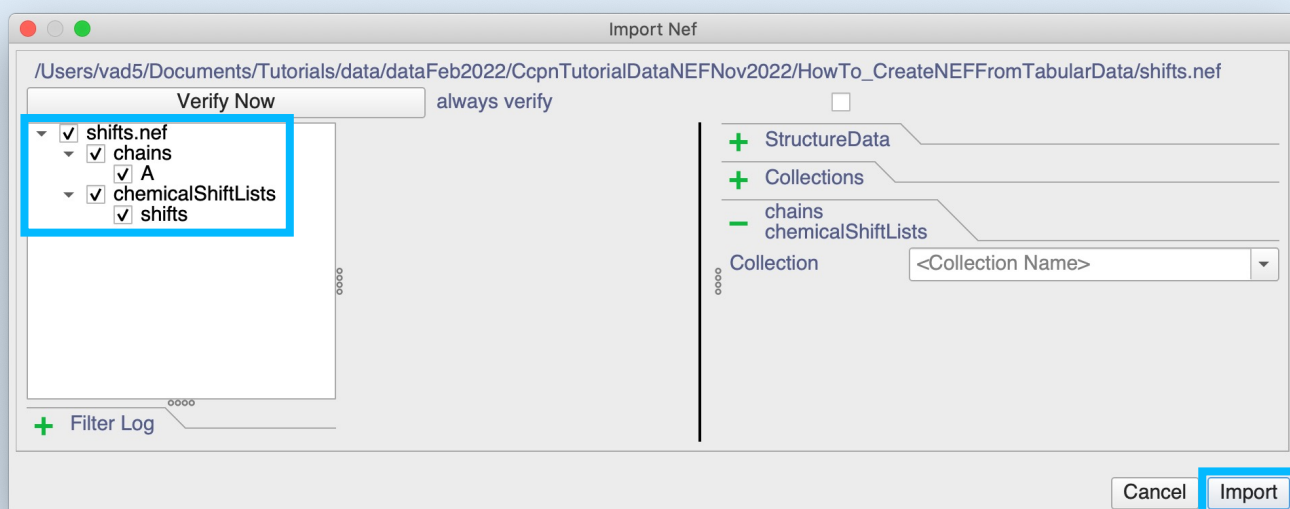
```
columns:      new order:

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.

ChemicalShift	ChemicalShift Value (ppm)	Value Error	NmrAtom	ResidueType	AtomName
CS:shifts.0	174.778	0.100	NA:A.3.ALA.C	ALA	C
CS:shifts.1	54.823	0.100	NA:A.3.ALA.CA	ALA	CA
CS:shifts.2	7.688	0.001	NA:A.4.MET.H	MET	H
CS:shifts.3	129.447	0.100	NA:A.4.MET.N	MET	N
CS:shifts.4	56.398	0.100	NA:A.4.MET.CA	MET	CA
CS:shifts.5	176.674	0.100	NA:A.4.MET.C	MET	C
CS:shifts.6	8.435	0.001	NA:A.5.LYS.H	LYS	H
CS:shifts.7	122.580	0.100	NA:A.5.LYS.N	LYS	N
CS:shifts.8	29.396	0.100	NA:A.5.LYS.CB	LYS	CB
CS:shifts.9	56.415	0.100	NA:A.5.LYS.CA	LYS	CA

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)