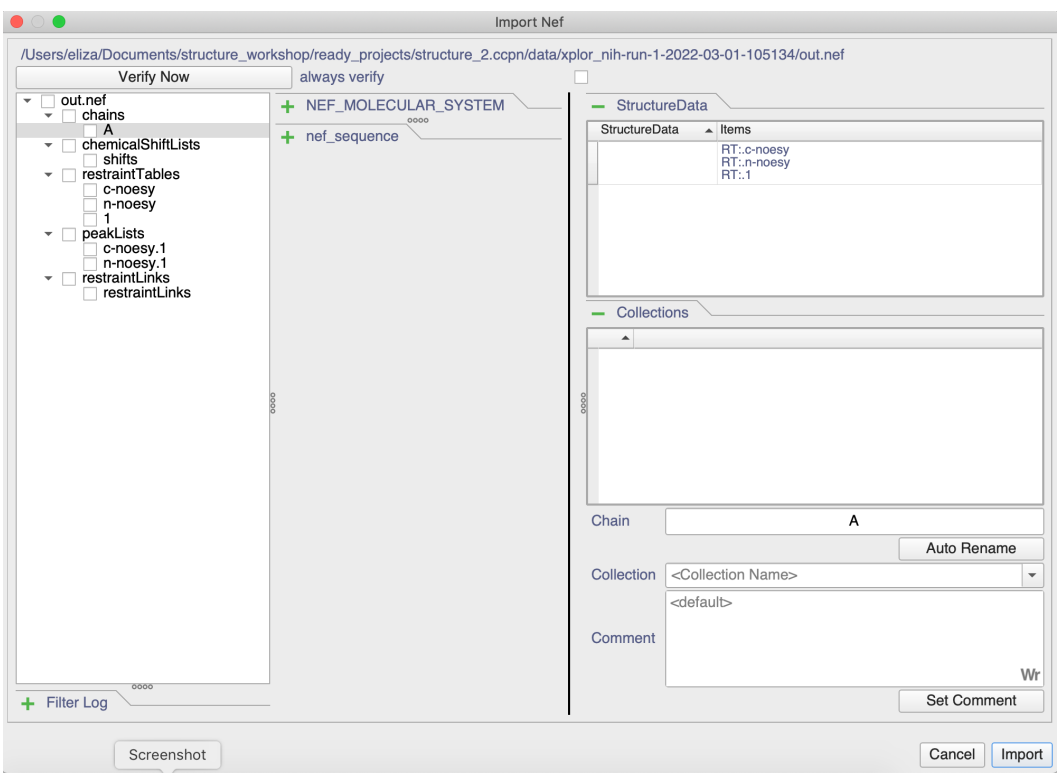
CCPN

CcpNmr Analysis Version 3

How To

Use NEF to import and export CcpNmr 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 guide you through the action of using the NMR Exchange Format, NEF, to move data from one CcpNmr project to another. This is only a practical example and not the main purpose of NEF, for documentation and other usages please visit:
https://github.com/NMRExchangeFormat/NEF.

In this How-To you will export the chain, chemical shift list and peak list from one project and import it to another using a NEF file. You can download example data for this How-To from our website at
https://ccpn.ac.uk/support/tutorials/#nef.

Start CcpNmr Analysis V3

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

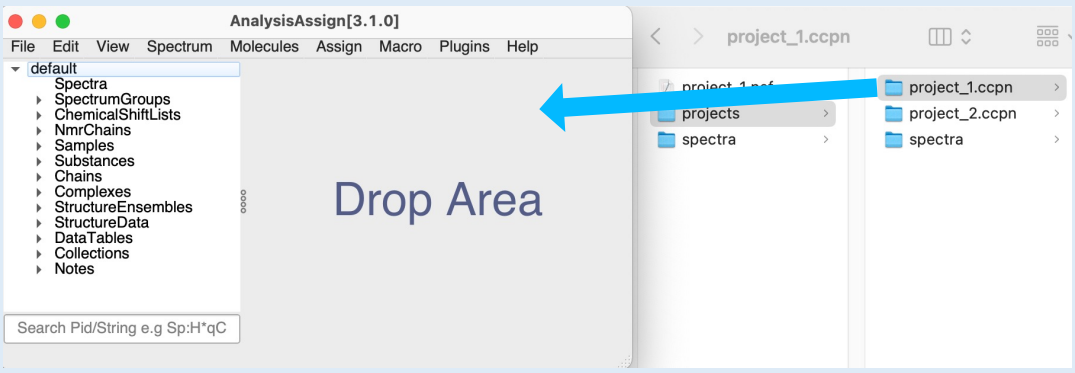
Windows users by double-clicking on the *assign.bat* file

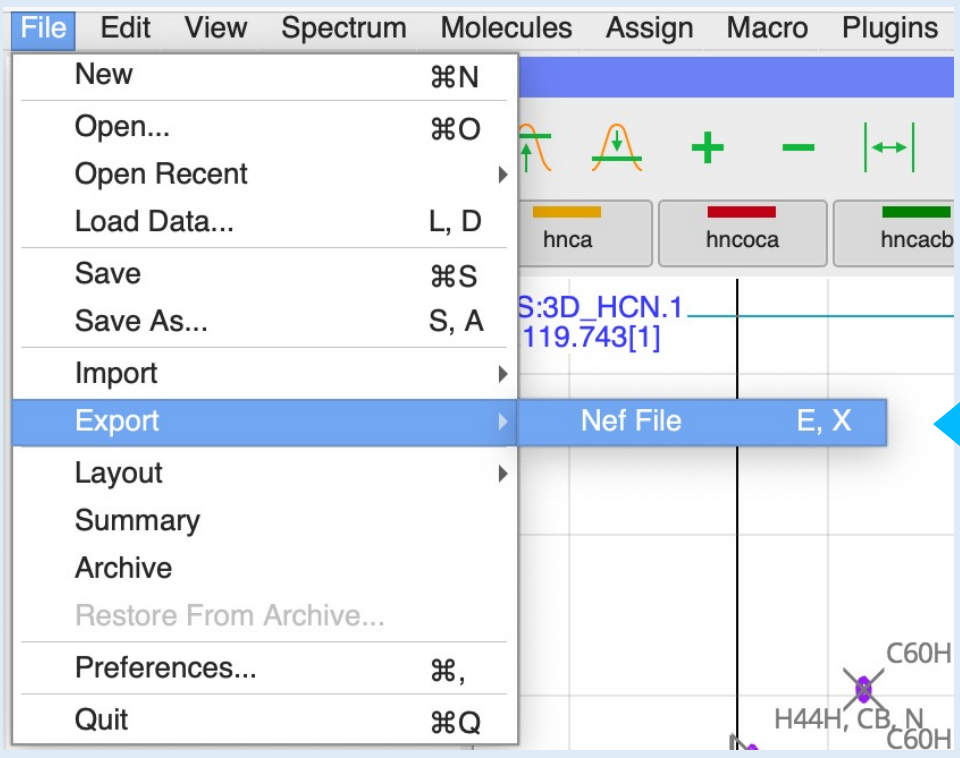
NMRbox users by using the terminal command *analysisassign*

How To 1

Export to NEF

Open project_1.ccpn





Shortcut **EX**

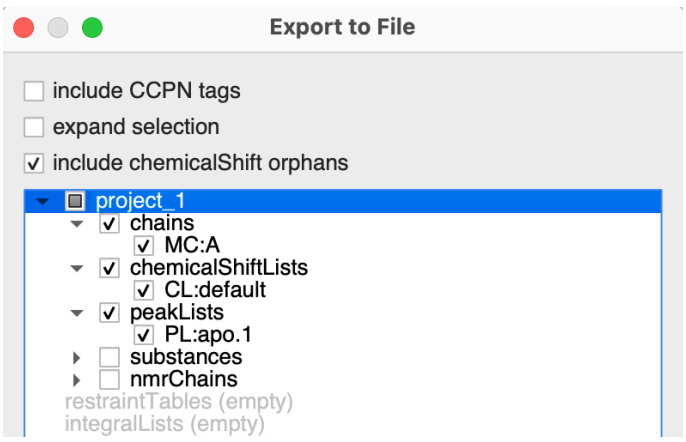
1A Open the project containing the data you want to export

- Open the project **project_1.ccpn** in the **projects** folder of the data provided.
- Open the NEF export popup:

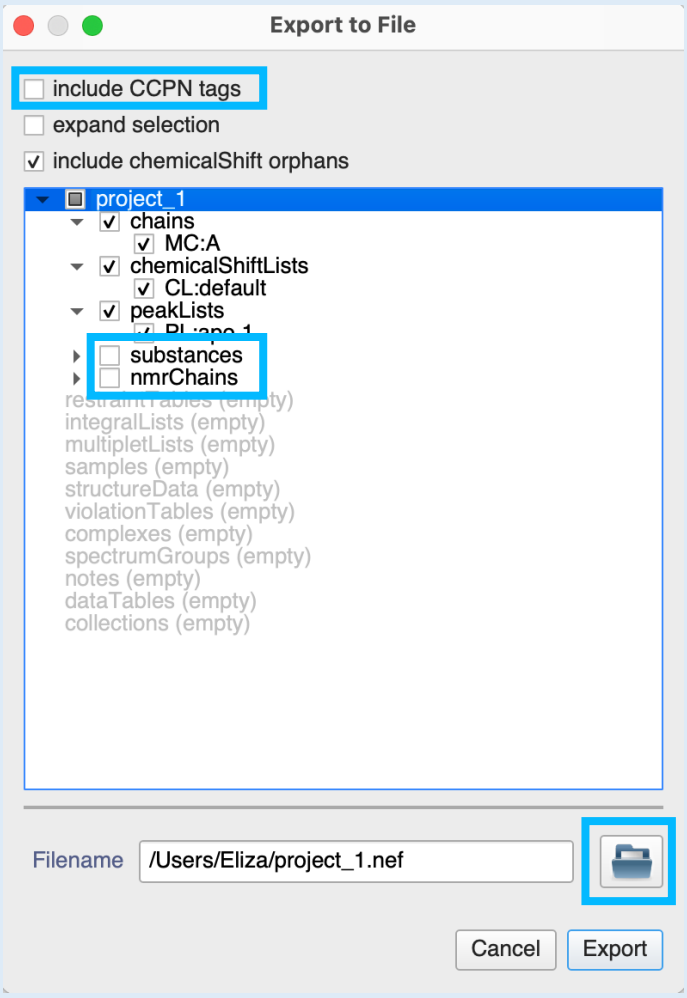
  Main Menu → File → Export → Nef File (or shortcut **EX**)

The NEF exporter dialog will appear.

- Expand the **chains**, **chemicalShiftLists** and **peakLists** branches



Export to NEF



1B Select exporting options

Elements not listed in the project are grayed out and not available for selection. We will export a Chain, ChemicalShiftList and PeakList (peak positions and heights/volumes) without the spectra.

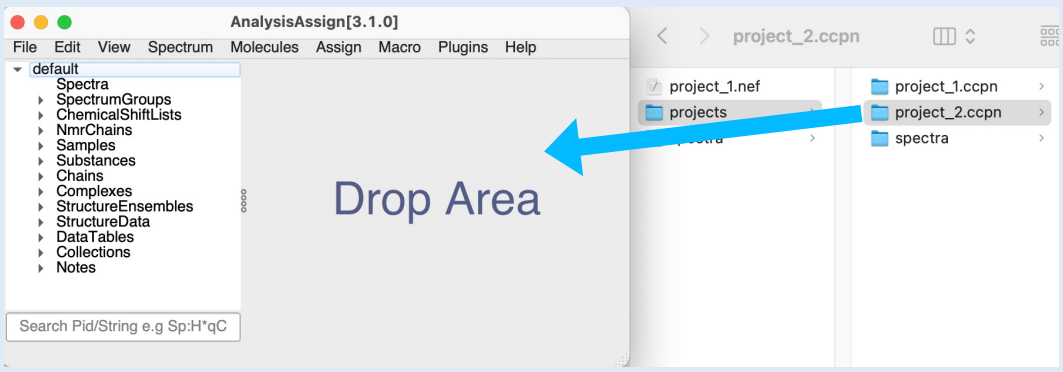
- Deselect **Include CCPN tags**
- Select
    - chains: **MC:A**
    - chemicalShiftLists: **CL:default**
    - peakLists: **PL:apo.1**
- Deselect **substances and nmrChains**

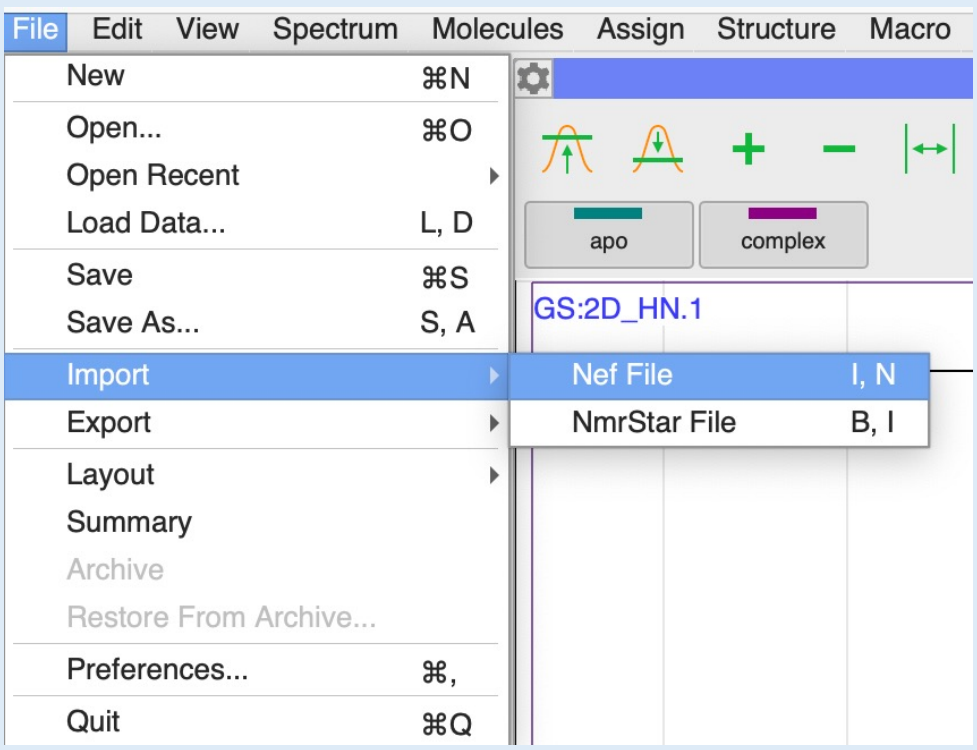
- Click on the folder icon to select the path where you want to save the NEF file.
- Click **Export**

Note: If you wish to export actual spectra (data locations), with all their display properties, you should select **Include CCPN tags**.

Import from NEF

Open project_2.ccpn





Shortcut **IN**

1c Import to a target project

- Open the project **project_2.ccpn**
- Open the NEF import popup with

  Main Menu → File → Import → Import Nef File (or shortcut **IN**)

A new File Dialog will appear.

- Select the previously saved NEF file
- Click **Open** to continue

A new popup will ask if you want to **Import** your NEF file or load it as a **New project**.

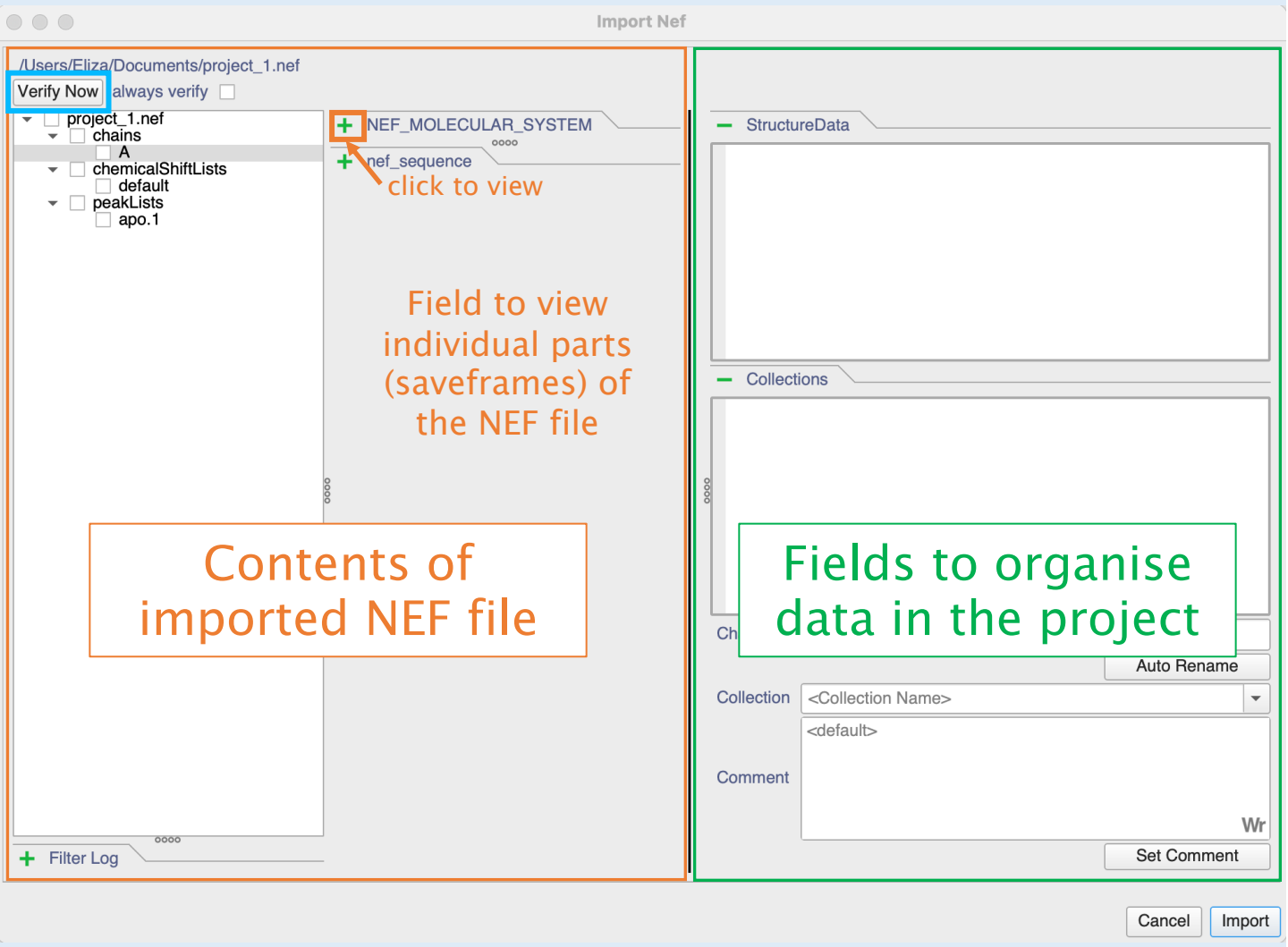
- Click **Import**

The **Import Nef** popup will open.

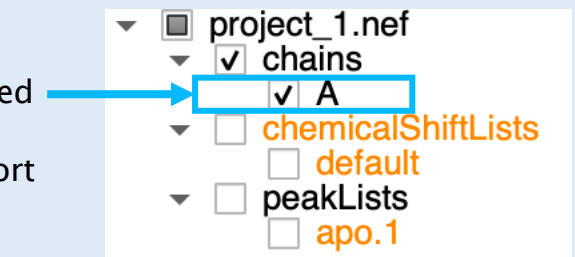
Import from NEF

project_2.ccpn

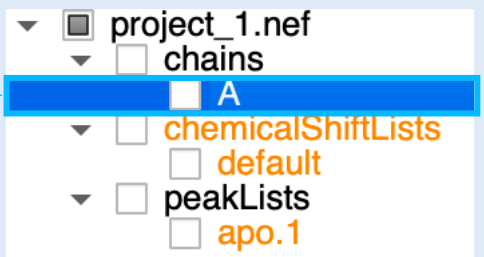
Nef importer



Ticked for import



Selected for edit



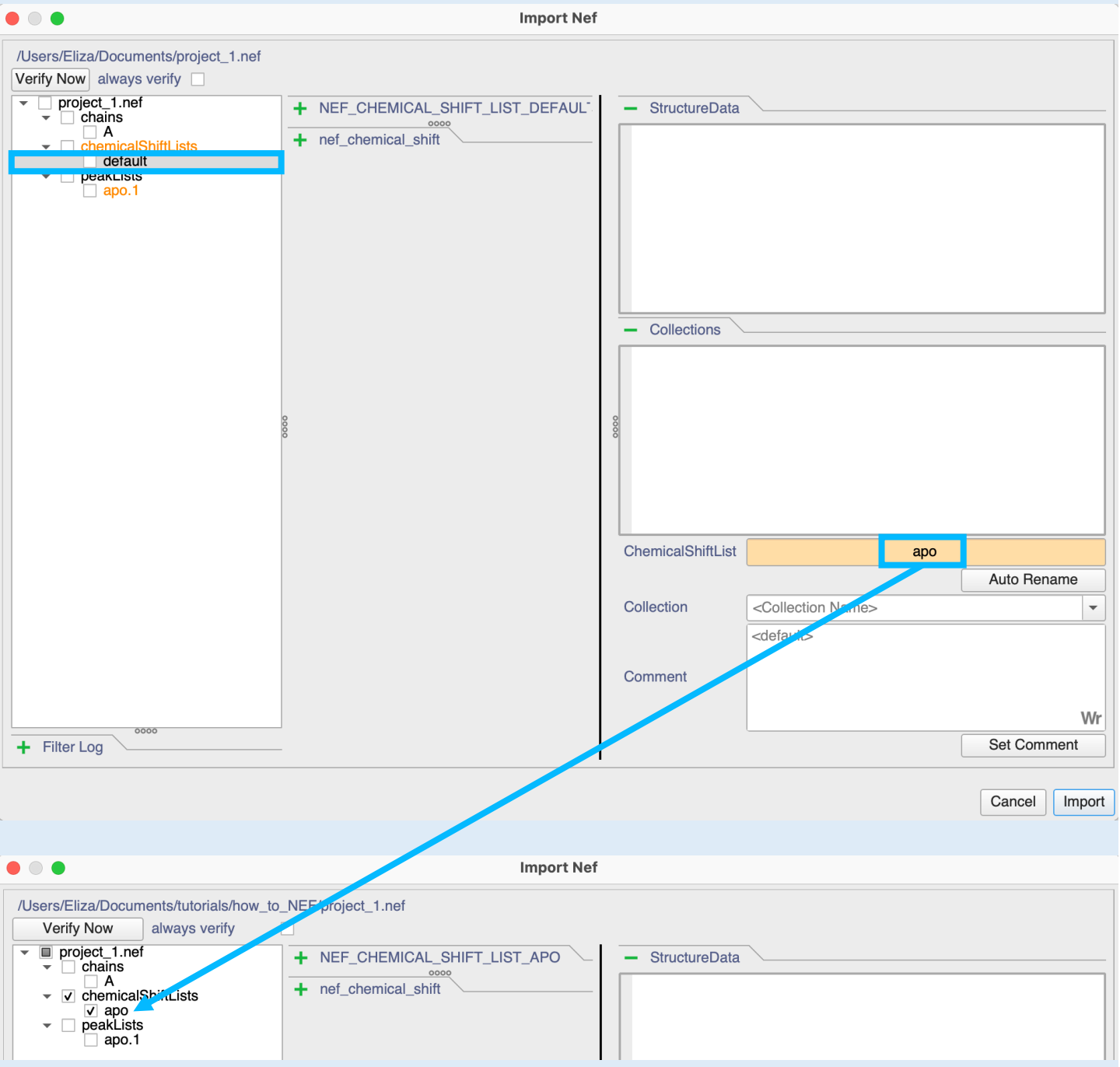
1D View incoming data from NEF file

- Click **Verify Now**

You will see that some elements are now coloured in orange, this indicates that objects with that name already exist in the project and their name must be changed before being adding to the project.

Import from NEF

Nef importer



1E Rename incoming items of data

- Click on the **default** chemicalShiftList on the left-hand side to select it for editing. It will appear in the right-hand side where it can be re-name, e.g. to **apo**. Press **Enter** to confirm the change. This will update the name on the left-hand side

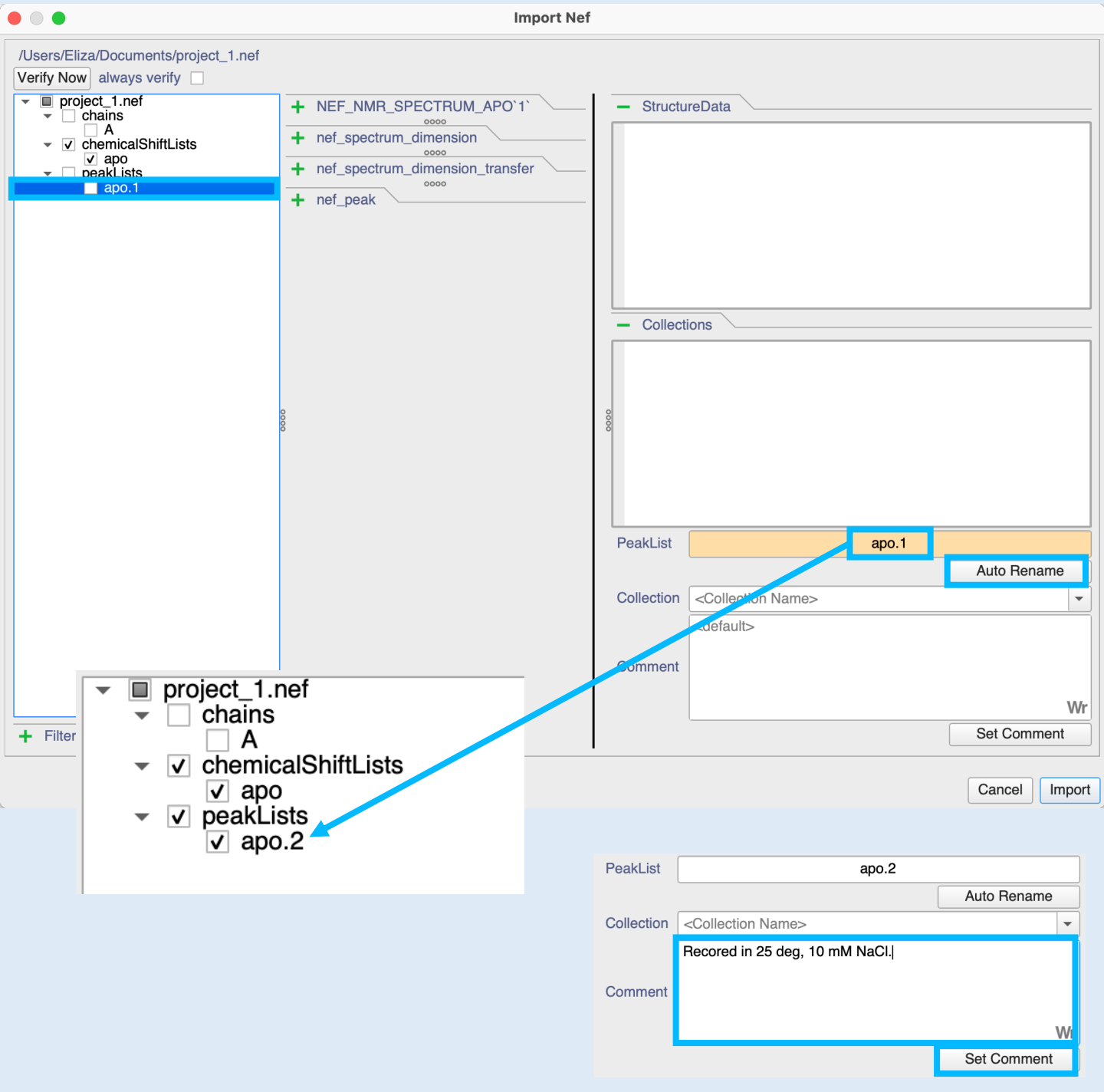
The chemicalShiftList has been now ticked automatically. If a name is edited, the software assumes this element is supposed to be imported into the project.

continued...

Import from NEF

project_2.ccpn

Nef importer



contintued… Rename incoming items of data

- Click on the **apo.1** peakList on the left-hand side to select it for editing

It will appear on the right-hand side.

- Click on the **Auto Rename** button.

This will change the peak list serial on the left-hand side and will tick the peak list automatically.

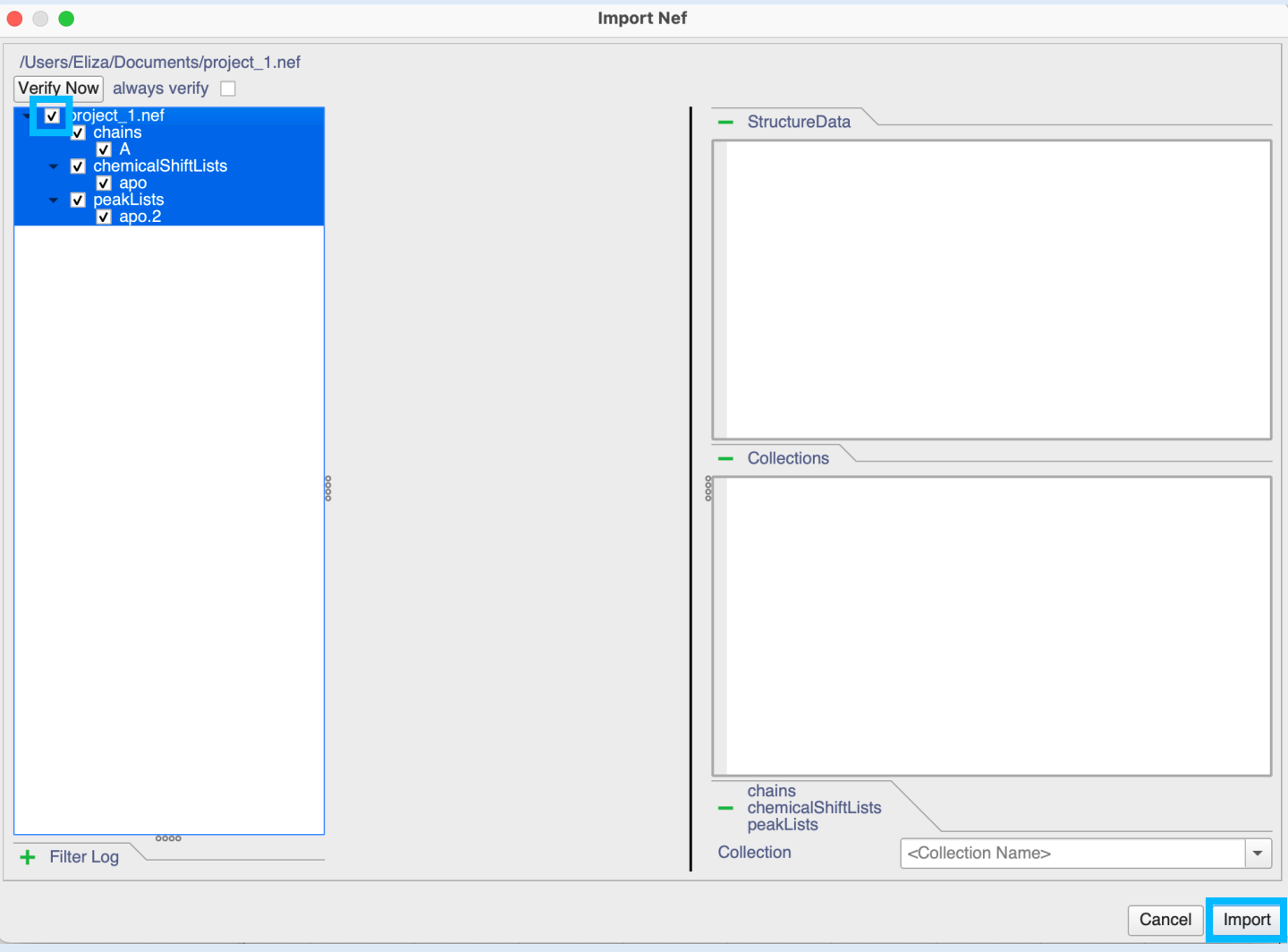
You can add a comment to any of the item of data you want to import when it is selected for editing:

- Type some text in the **Comment** box and click **Set Comment** to confirm.

Import from NEF

project_2.ccpn

Nef importer

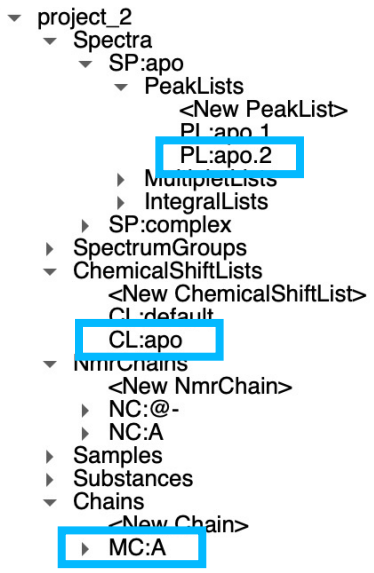


1F Import and inspect imported data

- Tick the box next to the **project_1.nef** to select the contents of an entire NEF file to be imported into your project.
- Click **Import**.

The newly imported items of data will appear in the sidebar.

Note that when you import a PeakList, then any PeakLabels (NmrAtoms) which are missing, will be automatically created and added to the project.



Contact Us

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support@ccpn.ac.uk

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

Cite Us

Skinner, S. P. *et al.* CcpNmr AnalysisAssign: a flexible platform for integrated NMR analysis. *J. Biomol. NMR* (2016). doi:10.1007/s10858-016-0060-y

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).