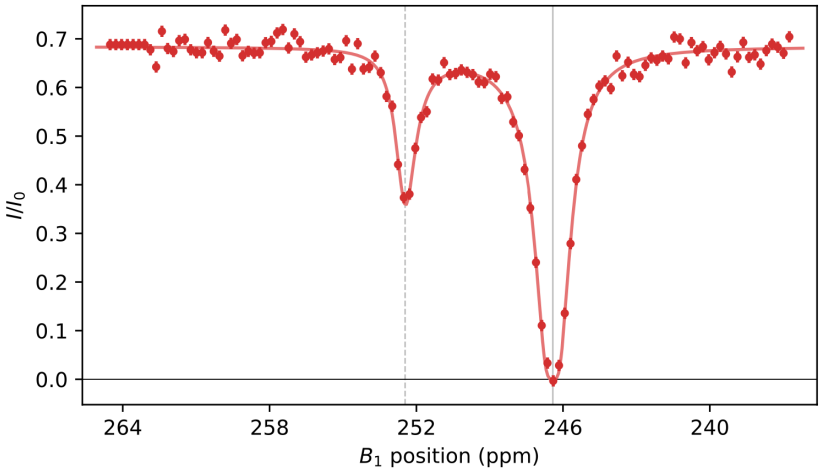
CCPN

CcpNmr Analysis Version 3

ChemEx
(beta testing)



Introduction

This tutorial will take you through the analysis of some dynamics data in the CcpNmr Analysis Version 3.5 pre-release. The functionality is still in the beta testing phase, so do please let us know about any bugs at support@ccpn.ac.uk or via our forum: https://forum.ccpn.ac.uk/.

We assume that you are already familiar with the basics of how the program works, e.g. by doing our Beginner Tutorial.

This tutorial focuses on how to use the new CcpNmr plugin interface to ChemEx, rather than on the underlying operation of ChemEx itself.

ChemEx is developed and maintained by Guillaume Bouvignies. For further details on ChemEx, refer to its main documentation and the associated publications available from the ChemEx webpage, https://gbouvignies.github.io/ChemEx/docs/welcome_to_chemex.

You are therefore expected to be familiar with the ChemEx program and its data structure before starting this tutorial.

You can download the example data to go with this tutorial from our website at https://ccpn.ac.uk/support/tutorials-for-analysisdynamics-pre-release/.

Example ChemEx datasets are available on its main GitHub page: https://github.com/gbouvignies/ChemEx/tree/main/examples.

The tutorial is divided into sections, each of them has a set of simple actions: you will see a descriptive image on top and a full description below. (Note that images are representative, and that there may be small differences between your setup and that shown in the tutorial.)

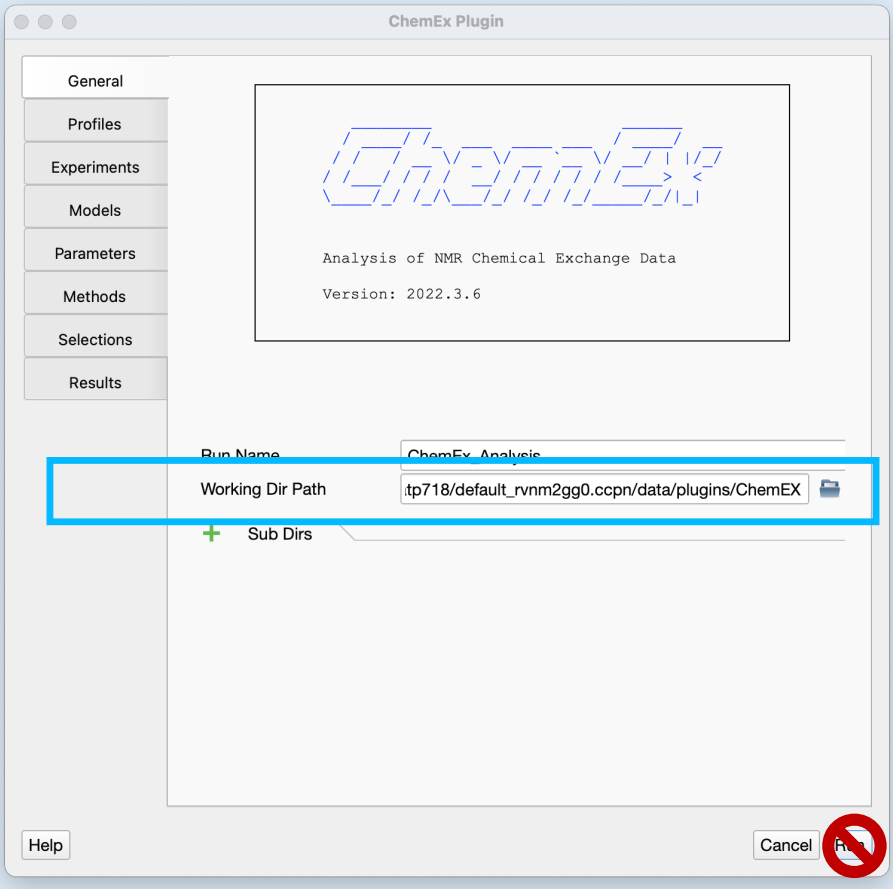
Contents:

Start CcpNmr Analysis V3

Apple/Linux users by using the terminal command *bin/assign* in the ccpnmr directory

Windows users by double-clicking on the *assign.bat* file in the bin directory of the ccpnmr directory

1 ChemEx Plugin



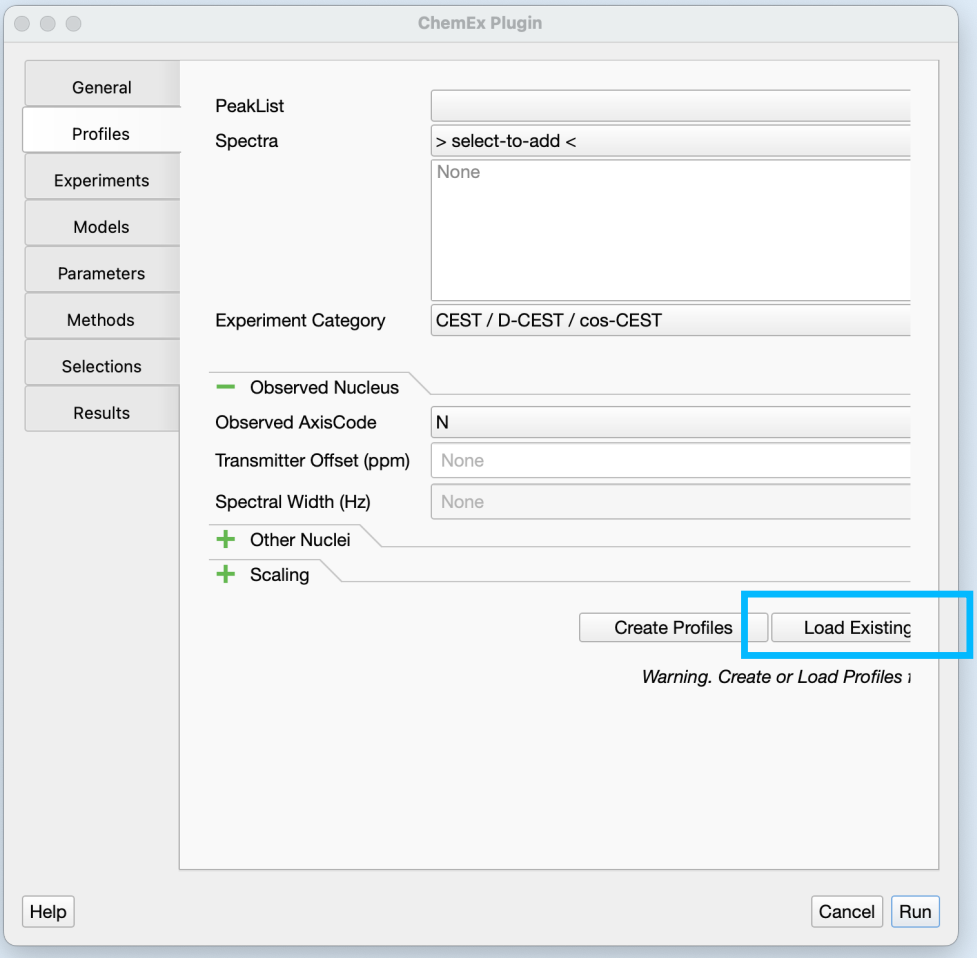
Always ensure that you are using the latest release. Updates can be run from the Help menu or from the Launcher.

1A Start ChemEx

Download and unpack the ChemEx demo data from https://ccpn.le.ac.uk/download/ccpnmr/v3TutorialData/ExchangeDemoData.zip

- Start AnalysisDynamics
- Go to **Main Menu → Dynamics → Run ChemEx** …
- The first tab is dedicated for the general paths. Set a run name.
- Set the Working Dir Path to the directory containing the Input Data, for example, the **ChemEx_Example1** dir from the demo dataset. (You can also drag and drop the folder to the entry widget)
- Leave the Sub Dir as default
- Do not press run!

1 ChemEx Plugin

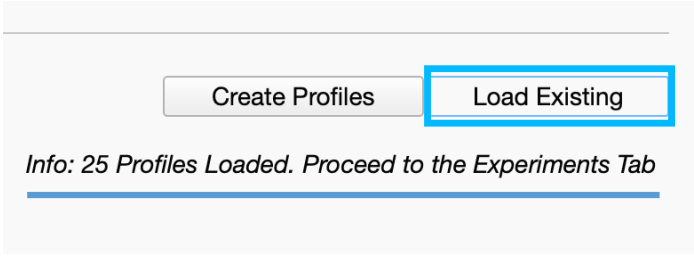


1B Load Profile

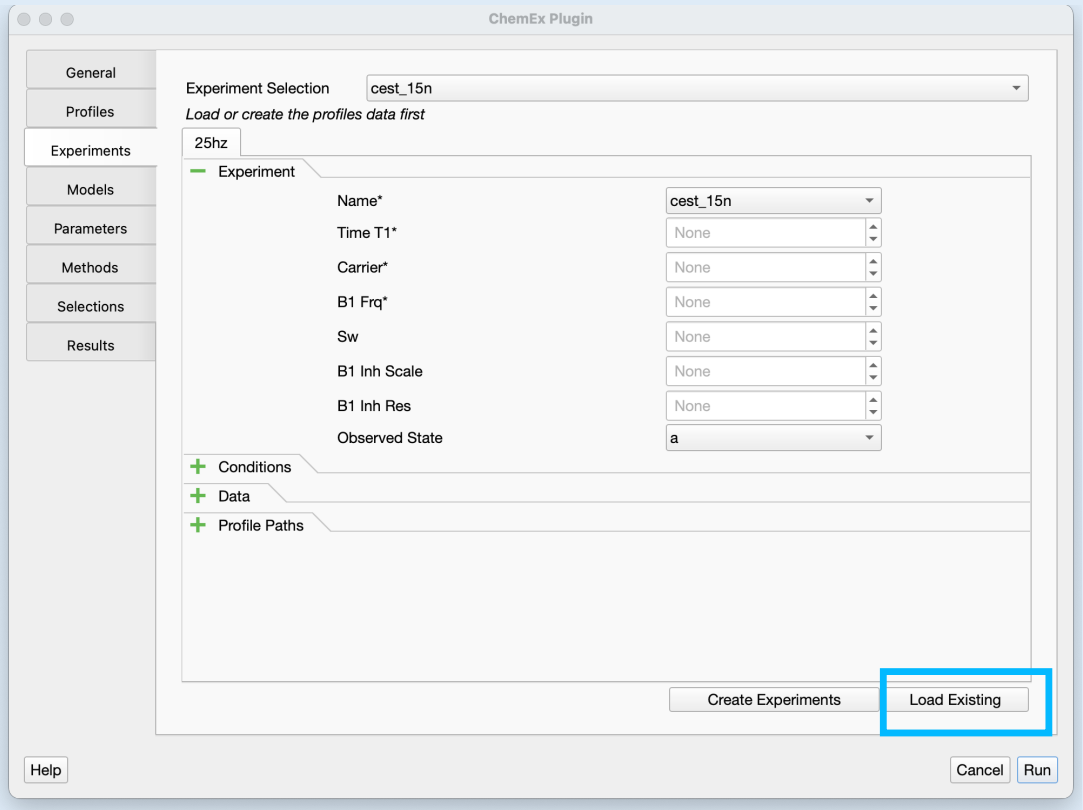
Select the Profiles tab.

For this tutorial we will use existing profiles.

Skip all the options and click: Load Existing



1 ChemEx Plugin



1C Load Experiments

After the profiles have been loaded, Click and move to the tab Experiments. This Experiment is for a Cest 15N analysis.

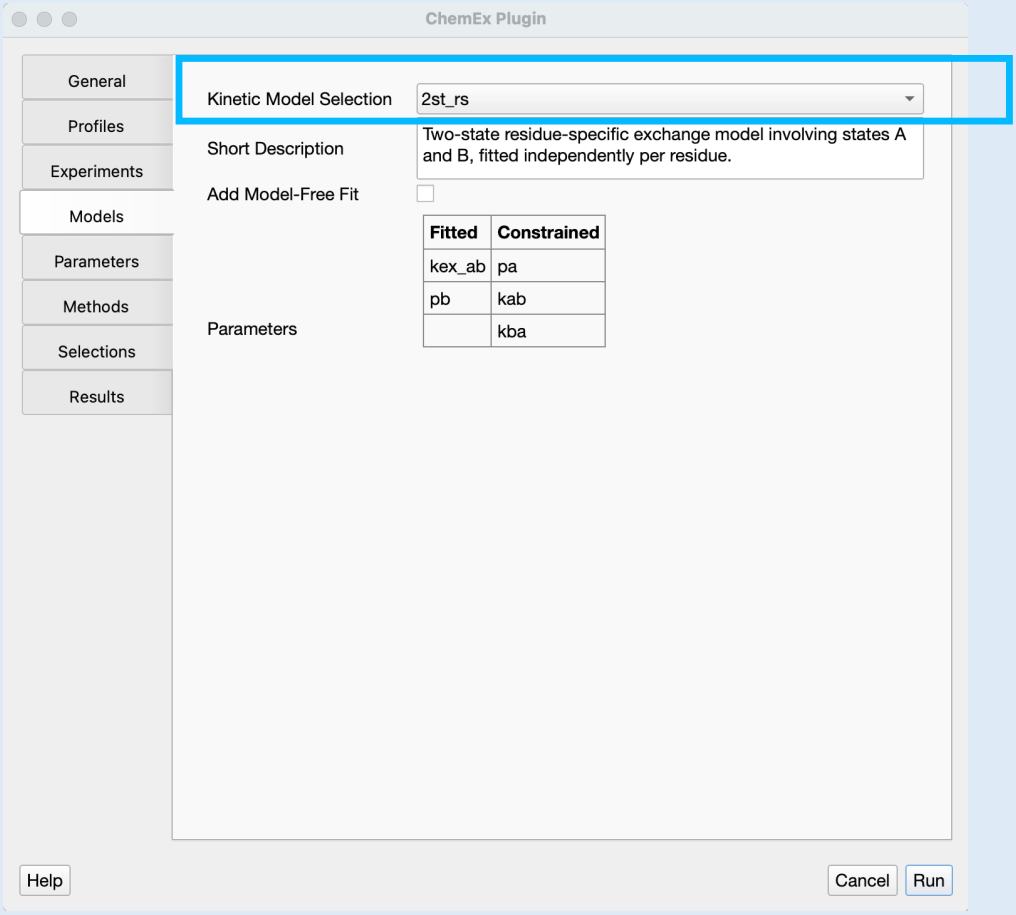
- Click Load Existing. This operation will load the TOML files from the ChemEx data directory and populate the various information.
  A new tab will be created for each field.

- Expand the Data section and ensure that the path points to your local data. It should be relative to the Experiment File i.e.: **..data/25hz** or the full absolute path to your data directory*.

More information is available at
https://gbouvignies.github.io/ChemEx/docs/experiments/cest/cest_15n

* Warning: ChemEx converts data paths to lowercase. On case-sensitive filesystems, paths containing uppercase letters may not resolve correctly. Ensure all file and directory names use lowercase, or verify that your filesystem is case-insensitive.

1 ChemEx Plugin



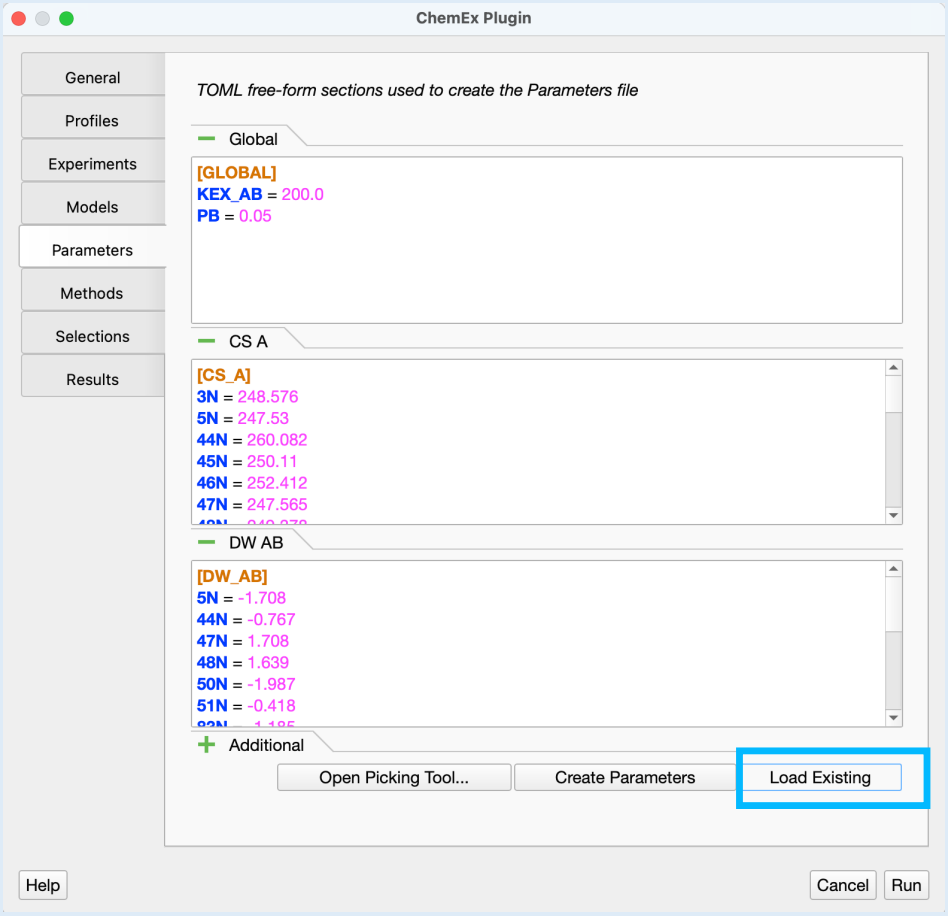
1D Model Selection

ChemEx let you select one Model per run.

For this tutorial we will run a two state Model. You can read the various supported models at https://gbouvignies.github.io/ChemEx/docs/user_guide/fitting/kinetic_models

- Select the 2st_rs

ChemEx Plugin

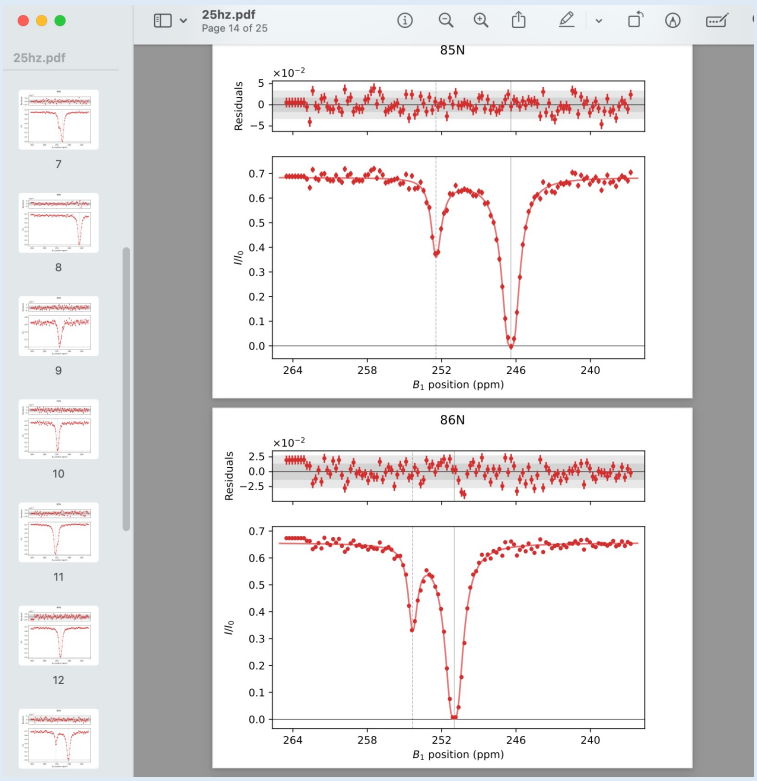


1E Load the Parameters

Next select the Parameters Tab. This tab will let load existing parameters or run the picking tool available within ChemEx to prepare them in a new TOML file.

- Click Load existing
- A new set of value will populate the TOML editors

ChemEx Plugin



1F Run

Skip the next two tabs, Methods and Selections for this tutorial

- Click Run

The calculation will run in the background. You will see the log directly in the console.

Once the calculation has finished, a new set of result files will appear in the working directory, including a PDF report of the fitting results.

Pdf is located at

/ChemEx_Example1/Results/All/Plots

```
  ________                              ______
 / ____/ /_  ___  ____ ___  / ____/ __
/ /   / __ \/ _ \/ __ `__ \/ __/ | |/_/
/ /___/ / / /  __/ / / / / / /____>  <
\____/_/ /_/\___/_/ /_/ /_/_____/_/|_|

Analysis of NMR chemical exchange data

Version: 2022.3.6

Loading datasets...
  • Reading Experiments/25hz.toml (cest_15n) ...
  • Reading Experiments/25hz.toml (cest_15n) -> 25 profiles

Reading default parameters...

Starting the fits...
  • Fit method -> leastsq
  • Running the minimization...

   ·····  Group 1_3 (1/25)  ·····

    Iteration           χ²     Reduced χ²
```

Contact Us

Website:
www.ccpn.ac.uk

Suggestions and comments:
support@ccpn.ac.uk

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

Cite Us

Mureddu L.G. et al. CcpNmr AnalysisDynamics: a unified framework for NMR dynamics data analysis. **(2026)**
https://doi.org/10.64898/2026.06.19.733360
Pre-print BIORXIV

See ChemEx webpage for preferred citations