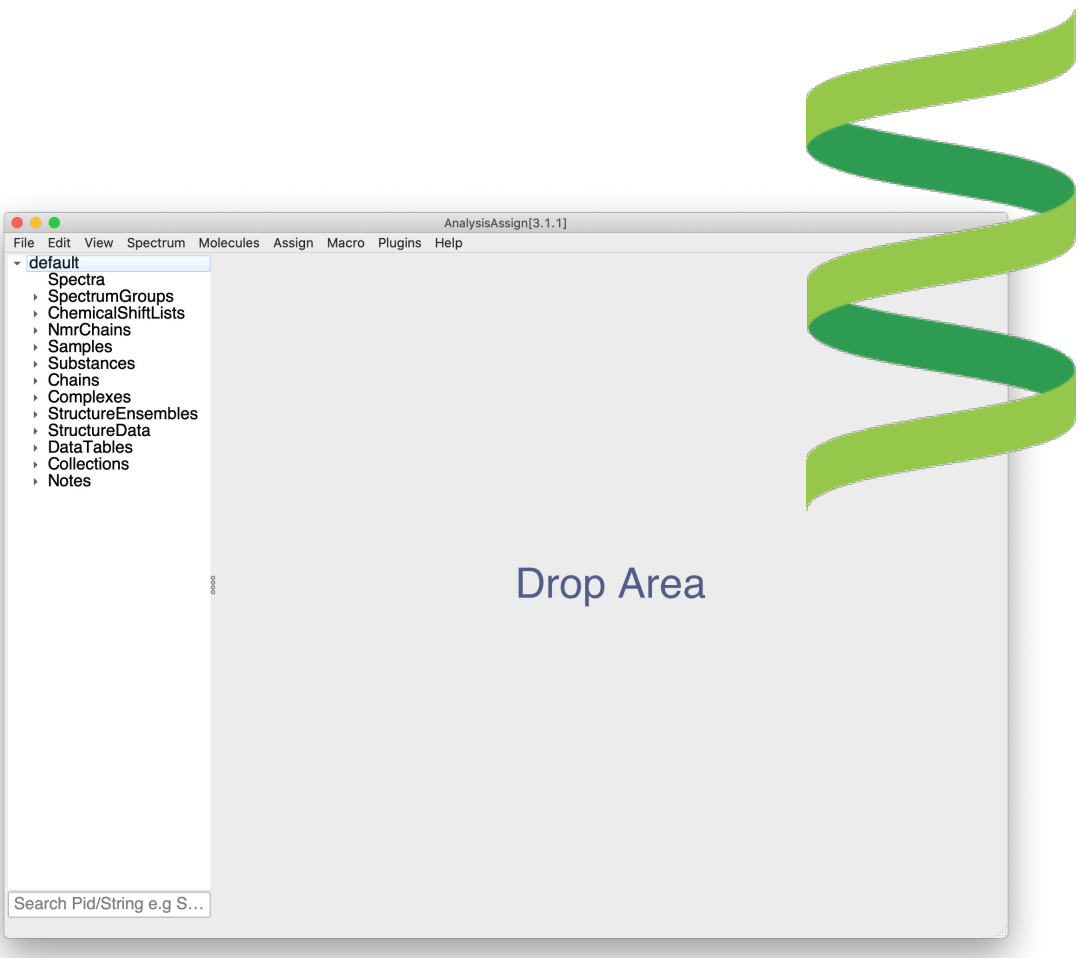
# BMRB / NMR-STAR Import



# Introduction

This tutorial will guide you through how to download an NMR-STAR format file from the BMRB, import it into a Analysis V3 Project and simulate a simple $^{15}$N-HSQC spectrum peak list.

Contents

1. BMRB Download
2. NMR-STAR Import
3. Simulate Peak List
4. Troubleshooting

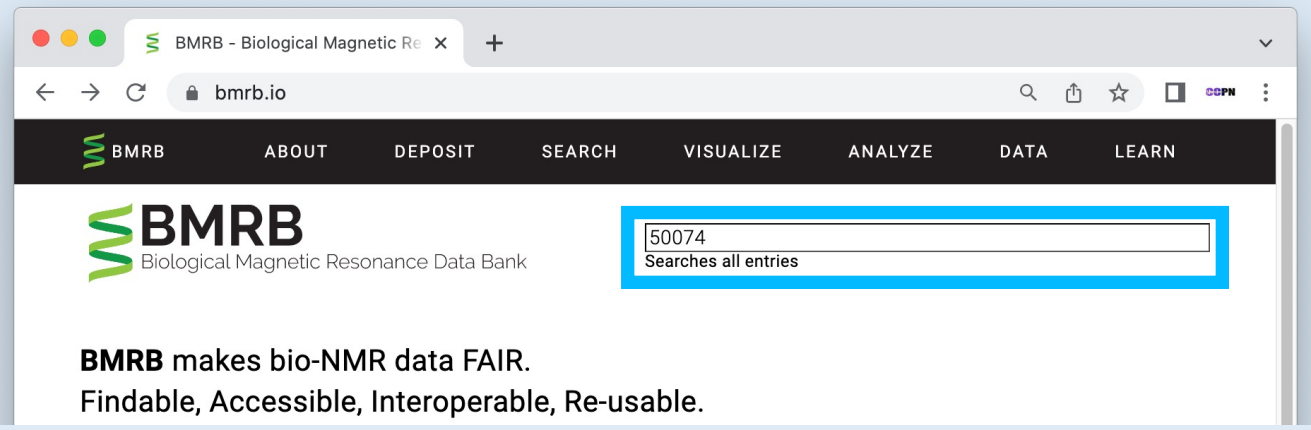
## Start CcpNmr Analysis V3

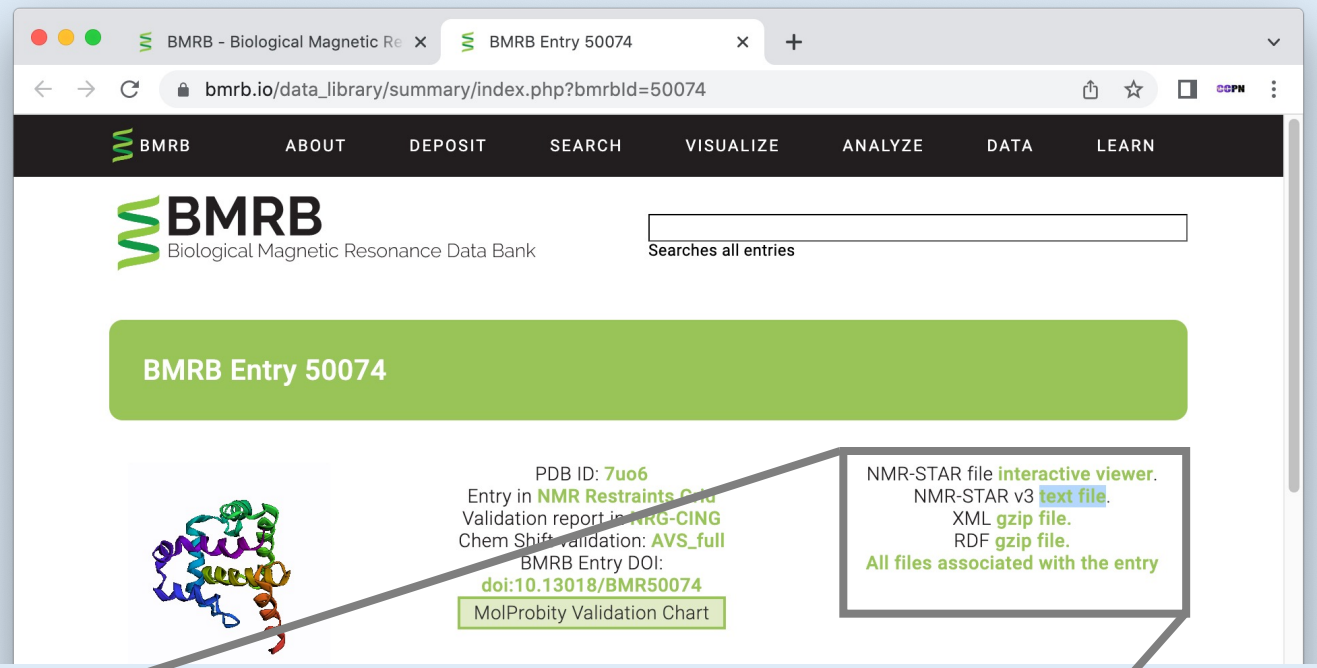
Apple users by double clicking the icon *CcpNmrAnalysis* or using the “linux” way (see below)

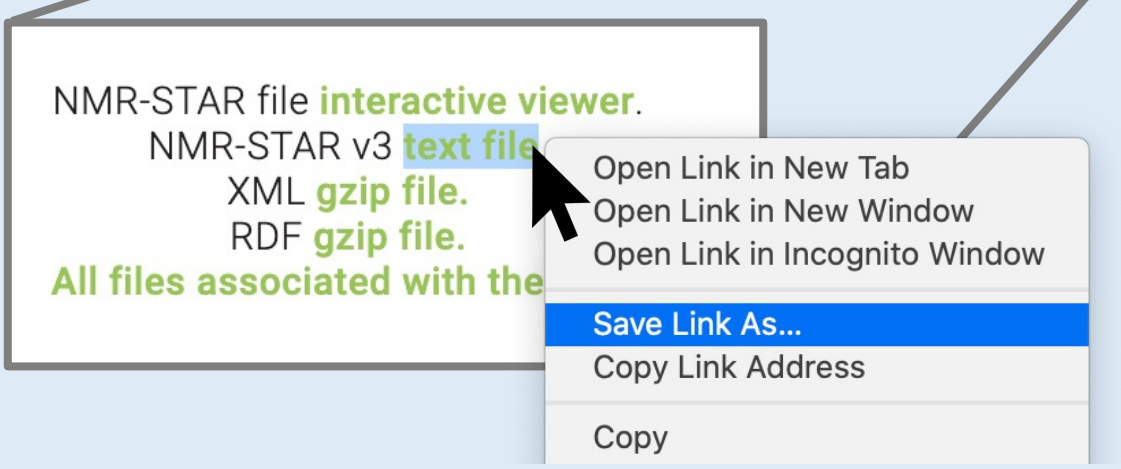
Linux users by using the terminal command: *bin/structure*

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

# 1 BMRB download



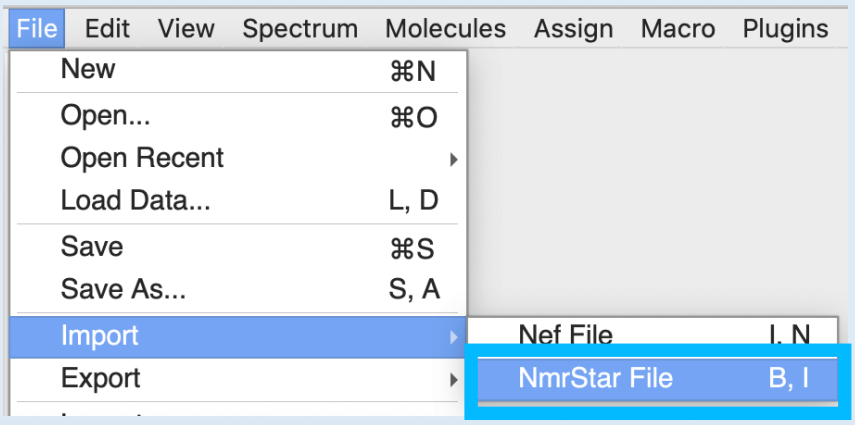



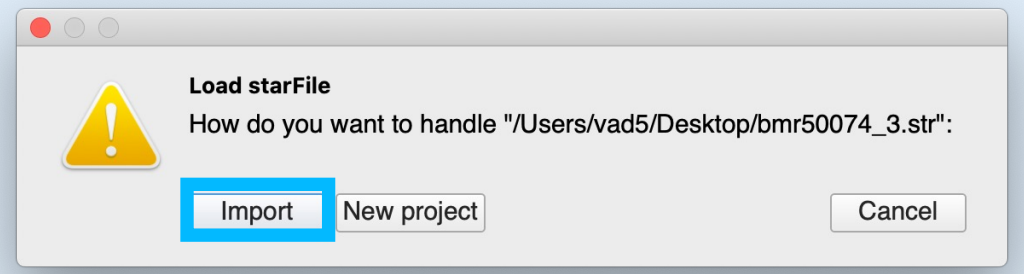

## 1A Download the NmrStar file from the BMRB

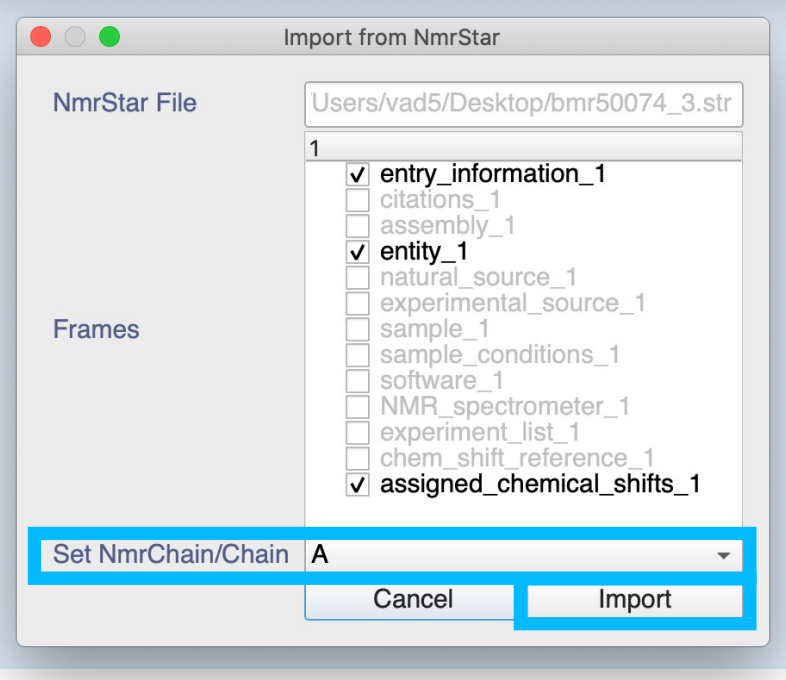
- In a web browser, go to **https://bmrb.io/**
- Enter **50074** into the search box (or another search term to bring up the BMRB entry of your choice).

- Next to **NMR-STAR v3**, right-click on **text file** to download the entry as a file.
- Make sure you save it with extension **.str**

# 2 NmrStar import




## 2A Import BMRB file into Analysis

- Go to **File → Import → NMStar File**, selecting the the **bmr50074_3.str** file

**OR**

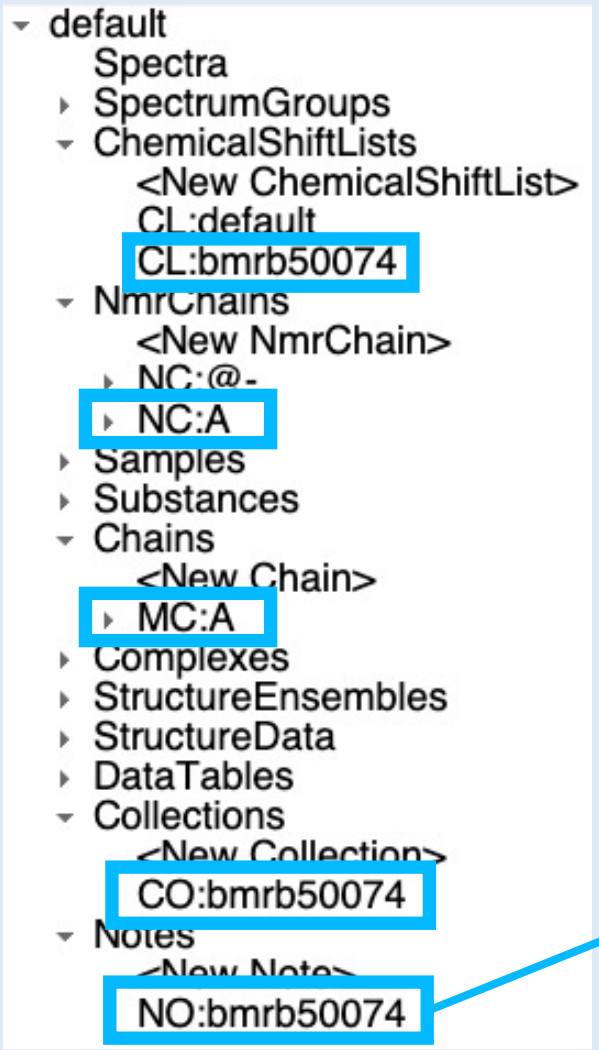
- Drag & Drop the **bmr50074_3.str** file into the Drop Area of the program.

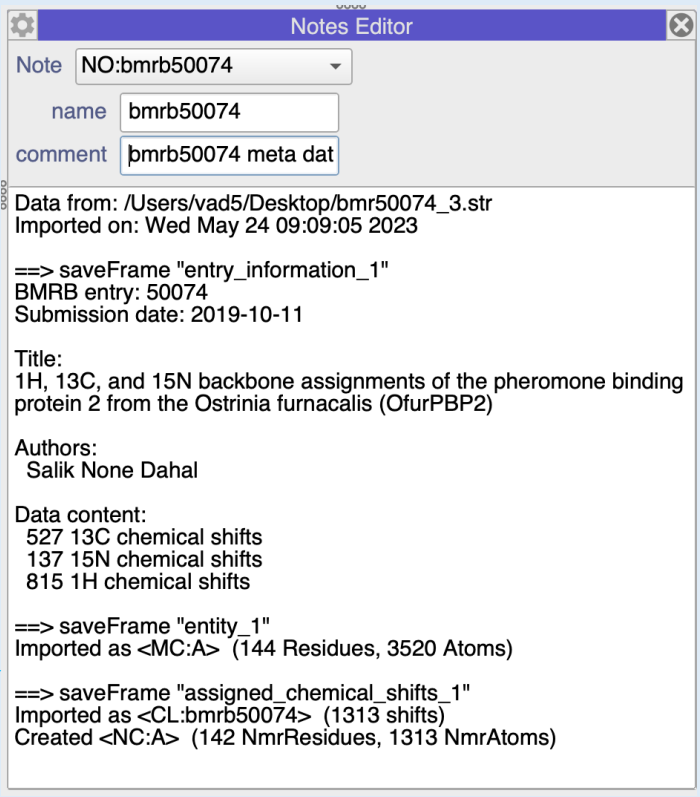
- When asked, select to **Import** the file.

The **Import from NmrStar** popup will open.

- Leave **entry_information_1, entity_1** and **assigned_chemical_shifts_1** ticked
- You can change the name of the Chain and NmrChain used to store the imported information in the **Set NmrChain/Chain** pulldown. Select **A** or the next available letter.
- Click **Import**.

# 2 NmrStar import




## 2B Inspect imported data

In the sidebar you will see the new data which has been imported:

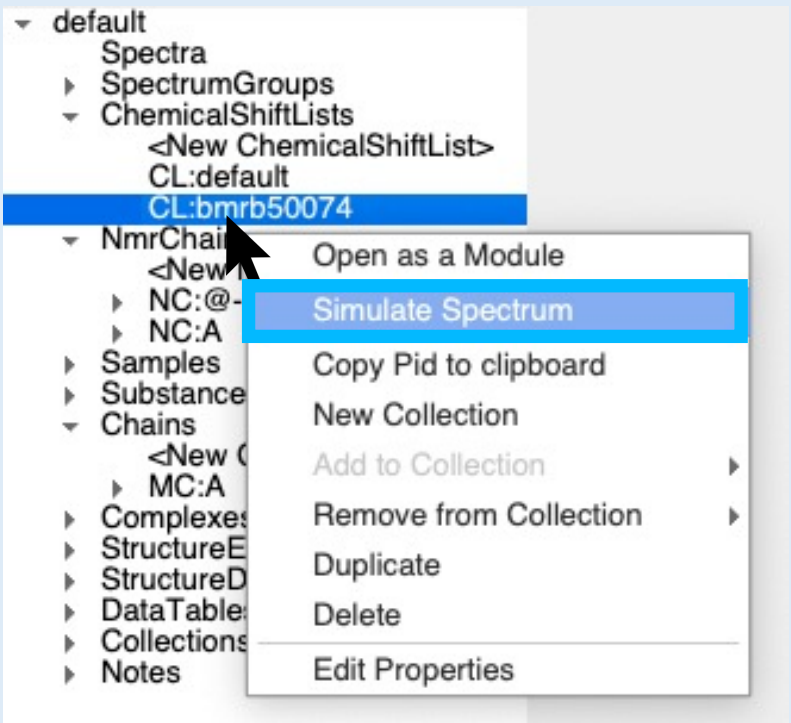
- ❖ A new ChemicalShiftList called **CL:bmrb50074**
- ❖ The new **NC:A** NmrChain containing all the atom labels
- ❖ The **MC:A** Chain containing the sequence of the molecule
- ❖ A Note called **NO:bmrb50074**. This contains the entry information from the NmrStar file.

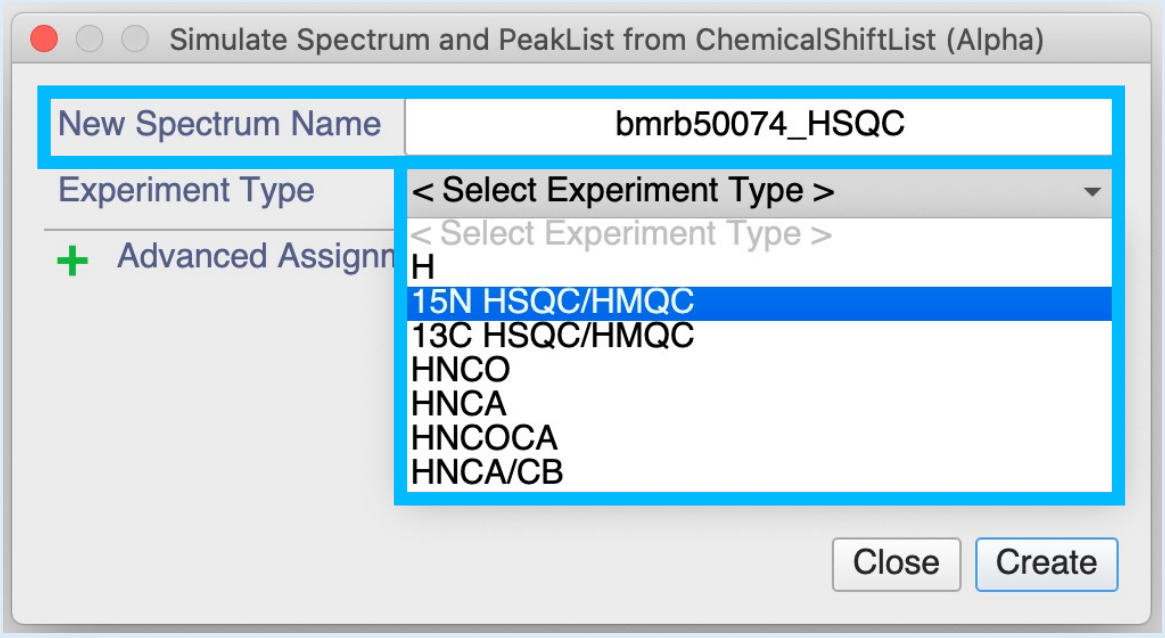
- If you wish, drag these items into the DropArea to open them as a module and inspect them.

- ❖ A Collection **CO:bmrb50074** has also been formed. This contains the other four items:

NO:bmrb50074
MC:A
CL:bmrb50074
NC:A

# 3 Simulate Peak List



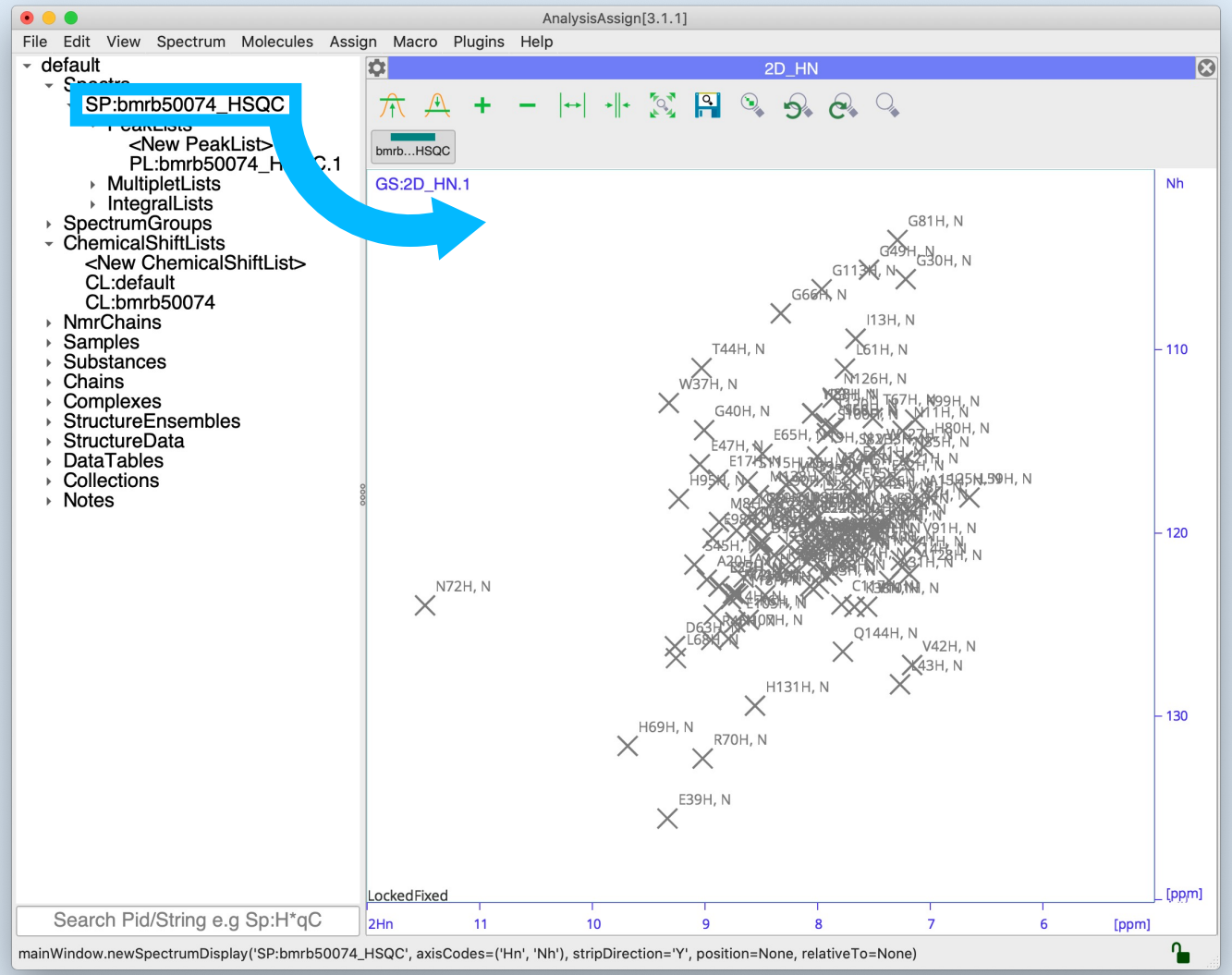




## 3A Simulate $^{1}H$-$^{15}N$ HSQC peak list

- **Right-click** on the **CL:bmrb50074** ChemicaShiftList in the sidebar.
- Click **Simulate Spectrum** which will bring up a dialog box.

- Change your **New Spectrum Name** to one of your choice, e.g. **bmrb50074_HSQC**.
- Select **15N HSQC/HMQC** in the **Experiment Type** pull down.
- Leave the **Advanced Assignment Options** as they are.
- Click **Create**.

# 3 Simulate Peak List




## 3B View $^{1}H-^{15}N$ HSQC peak list

You will see a new item added to the Spectra part of the sidebar: **SP:bmrb50074_HSQC**. This is an empty dummy spectrum that has been created to contain the $^{1}H-^{15}N$-HSQC PeakList which we have just created based on our imported shifts.

- Expand the **SP:brmb50074_HSQC** spectrum in the sidebar
- **Drag** the **SP:brmb50074_HSQC** spectrum into the DropArea.

You will see that the spectrum does not contain any contours, as we have only simulated the peaks and not the contours.

If you add another spectrum to your project, you can now copy the PeakList we have just created to that spectrum with **Spectrum → Copy PeakList** (shortcut **PL**) or by dragging the PeakList from the sidebar onto another (HN) spectrum.

# Contact Us

**Website:**
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**Suggestions and comments:**
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# Cite Us

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