

simpleNMRbrukerTools

A set of Python tools to use simpleNMR under Bruker NMR TopSpin ($\geq 4.5.0$).

Prerequisites

Before installing simpleNMRbrukerTools, ensure you have:

- **Python 3** installed for TopSpin 4.5.0
- **Bruker-TopSpin Python libraries* installed (follow the Bruker Python 3 API in Jupyter notebook PDF)
- Access to the Bruker/TopSpin Python3 environment

Installation

1. Download the Repository

1. **Open a terminal** and activate the Bruker/TopSpin Python3 environment
2. Clone or download the `simpleNMRbrukerTools` repository from GitHub by copying the command below and running it in the terminal window at a suitable directory location on your harddrive:

```
git clone https://github.com/EricHughesABC/simpleNMRbrukerTools.git
```

2. Install the Package into the Topspin Python 3 site-packages folder

1. Again, if not already done so, **Open a terminal** and activate the Bruker/TopSpin Python3 environment
2. **Navigate** to the `simpleNMRbrukerTools/simpleNMRbrukerTools` folder:

```
cd simpleNMRbrukerTools/simpleNMRbrukerTools
```

3. **Install** using pip:

```
pip install .
```

3. Setup TopSpin Integration

1. **Ensure TopSpin is running**
2. **Run the topspin setup command** in your terminal:

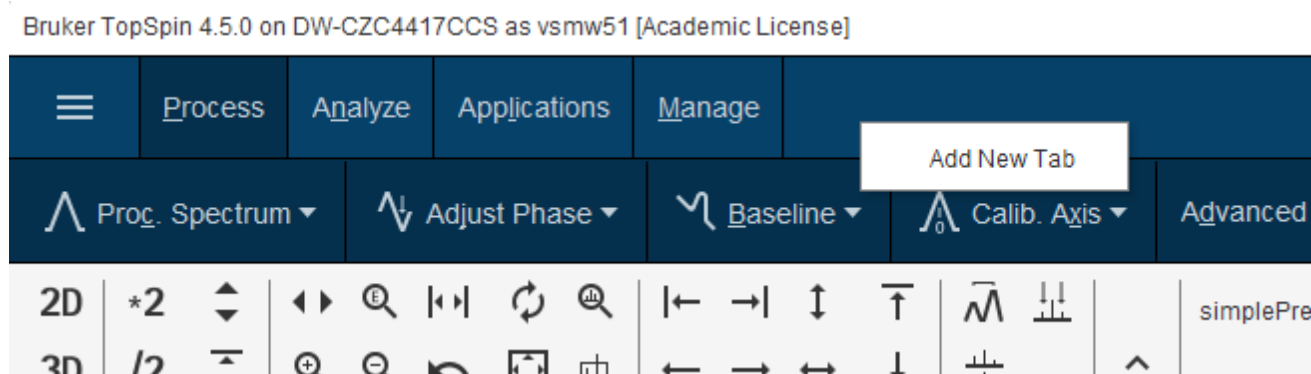
```
setup-topspin
```

This installs the main program into the Python 3 Topspin user directory and installs the TopSpin flowbar integration files.

TopSpin Flowbar Configuration

Add simpleNMR Tab to Flowbar

1. **Right-click** on the TopSpin flowbar menu to add an new tab:



2. **Fill in the empty dialog** that appears:

The 'User-Defined Tab' dialog box is shown. It has a title bar with a close button. The main area contains instructions: 'Set up user-defined Tab to be appended to the standard Tabs. Press Help for details. An example is given in parentheses.' Below this is a table with three columns: 'Tab ID (MY_T1T2_TAB)', 'Tab Text (T1 Fit)', and 'Flowbar File (t1_flowbar)'. The table has one empty row for input. At the bottom right are three buttons: 'OK' (with a green checkmark), 'Cancel' (with a red X), and 'Help'.

3. **Complete the dialog** with the required parameters and click **OK**:

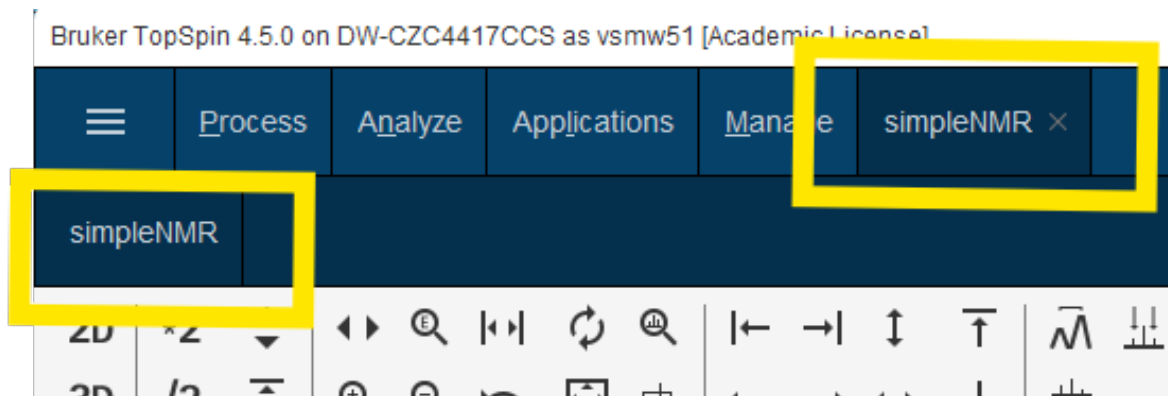
The 'User-Defined Tab' dialog box is shown with the fields filled. The 'Tab ID' field contains 'simpleNMR', the 'Tab Text' field contains 'simpleNMR', and the 'Flowbar File' field contains 'simpleNMR.prop'. The 'OK' button is highlighted with a green checkmark.

4. Topspin may need to be restarted to complete the installation.

Verification

After successful configuration, you should see:

- The new **simpleNMR menu item** in the Flowbar menu system
- A **button to start simpleNMR** directly from TopSpin



Troubleshooting

Common Issues

- **Installation fails:** Verify you're using the correct Bruker/TopSpin Python3 environment
- **setup-topspin command not found:** Ensure the package installed correctly with `pip list | grep simpleNMRbrukerTools`
- **Flowbar integration not working:** Make sure TopSpin is running before executing `setup-topspin`

Support

For issues and questions:

- Check the [Issues](#) page
- Refer to the Bruker Python3/Jupyter tutorial documentation
- Send an email to simpleNMR@gmail.com for direct assistance

License

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Contributing

If you are interested in helping please get in touch. Fork the project and submit an update. If you have comments or suggestions get in touch via email simpleNMR@gmail.com