How to set up an Anaconda environment for DNN pureshift

- Download the GitHub repository
- Open terminal (for Linux/Mac) or Anaconda prompt (for Windows) in the downloaded folder
- Create a conda environment for the environment.yml file; for example, the following command will create an environment named "pureshift"

  conda env create –f environment.yml

- Then the new environment, **pureshift**, can be activated with the command

  conda activate pureshift

- In the terminal, type ./run.sh (Linux/MAC) or run.bat in the anaconda prompt (Windows OS), and the output spectra will be stored as a .pdf file, with all individual spectra in the output folder in .csv format.

How to use DNN pureshift module

run.sh/ run.bat looks like the following,

```
python .pureshift \
        --spin_echo 'NMR/Kanamycin/3/' \
        --psyche 'NMR/Kanamycin/1002/'\
        --output 'pred' \
        --phase 0 \
        --p0 -125.0 \
        --p1 355.0 \
        --pp0 90.4 \
        --pp1 295.0 \
        --clear_phase 0 \
        --scaling 20 \
        --ver_scale 1.0 \
```

Arguments available in the DNN pureshift

Argument	Compulsory / Optional	Purpose	Remarks
--spin_echo	Compulsory	Path of spin-echo spectra	Example: --spin_echo 'NMR/Kanamycin/3/'
--psyche	Optional	Path of PSYCHE spectrum	Example: --psyche 'NMR/Kanamycin/1002/' **if PSYCHE is not available delete this line**
--output	Compulsory	The output folder name where the processed spectra will be saved in .csv format	Example: --output 'pred' It can accept any string variable
--clear_phase	Optional	Resets all phase values to 0.0 in all spectra	Example: --clear_phase 0 Always begin with --clear_phase 1 for each new sample analysis For any new sample or while performing phase correction, if things go out of control, --clear_phase 1 will reset all phases to 0.0
--phase	Optional	if phase correction is required set --phase = 1, else --phase = 0 (it is also the default and generates pure shift)	Example: --phase 1 Always begin with --phase 1 for every new sample analysis Once the phase correction is completed, set --phase 0 for DNN pure shift analysis
--p0	Optional	Spin-echo spectra zero-order phase that needs to be changed It is only used with --phase 1	Example: --p0 125.0 We may not be able to change the zero-order phase by 125.0 in a single step; however, this can be accomplished over multiple steps. For example, consider a phase change of 70.0 in the first step and only 55.0 in the next.
--p1	Optional	Spin-echo spectra first-order phase that needs to be changed It is only used with --phase 1	Similar to the --p0
--pp0	Optional	PSYCHE zero-order phase that needs to be changed It is only used with --phase 1	Similar to the --p0
--pp1	Optional	PSYCHE first-order phase that needs to be changed	Similar to the --p0

		It is only used only --phase 1	
--scaling	Optional	Vertical space between the spectra can be changed using this argument	Example: --scaling 20 To plot the spectra without any vertical overlap, this argument can be used For example, while plotting Kanamycin spectra, we found that --scaling 20 (also the default setting) clearly separate the spectra
--ver_scale	Optional	This helps in changing the intensity of spectra	Example: --ver_scale 1.0 The default value is 1.0 (for DNN pureshift processed spectrum) During plotting, the intensity of DNN pureshift is raised by 1.0, PSYCHE by 64.0, and conventional by 4.0

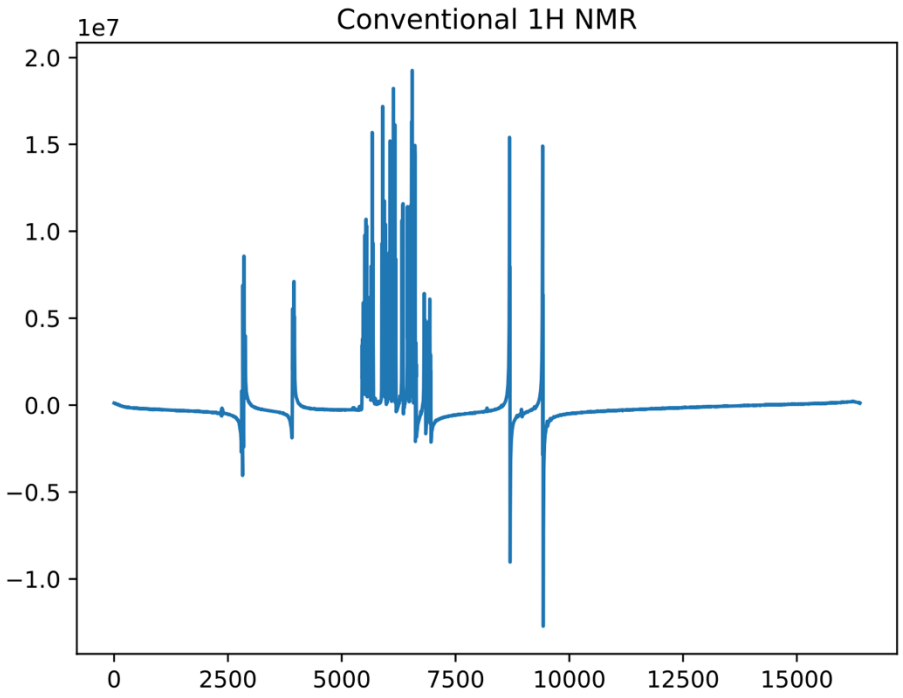
How to modify the arguments in run.sh/run.bat file

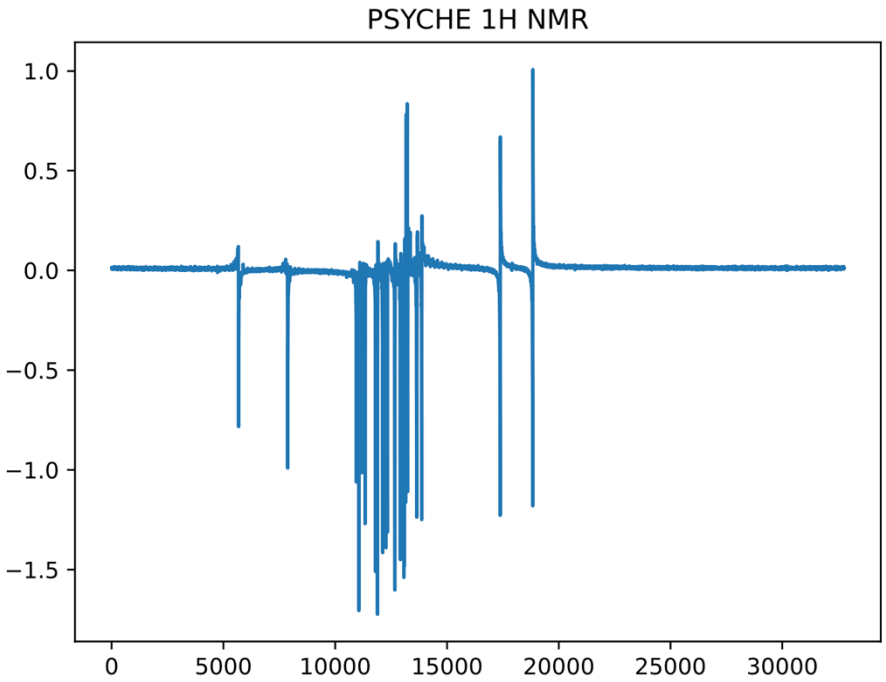
1. As an initial step, reset all phases to zero with **--clear_phase 1**

   ```
   python .pureshift \
           --spin_echo 'NMR/Kanamycin/3/' \
           --psyche 'NMR/Kanamycin/1002/' \
           --output 'pred' \
           --phase 0 \
           --p0 0.0\
           --p1 0.0 \
           --pp0 0.0 \
           --pp1 0.0 \
           --clear_phase 1 \
           --scaling 20 \
           --ver_scale 1.0 \
   ```

2. Along with **--phase** 1, set all of the **p0, p1, pp0, and pp1 to 0.0**, and the spectra will be plotted without any phase correction values. It aids in determining which phase values need to be adjusted. The resulting spectra are shown below.

   ```
   python .pureshift \
           --spin_echo 'NMR/Kanamycin/3/' \
           --psyche 'NMR/Kanamycin/1002/' \
           --output 'pred' \
           --phase 1 \
           --p0 0.0\
           --p1 0.0 \
           --pp0 0.0 \
           --pp1 0.0 \
           --clear_phase 0 \
           --scaling 20 \
           --ver_scale 1.0 \
   ```

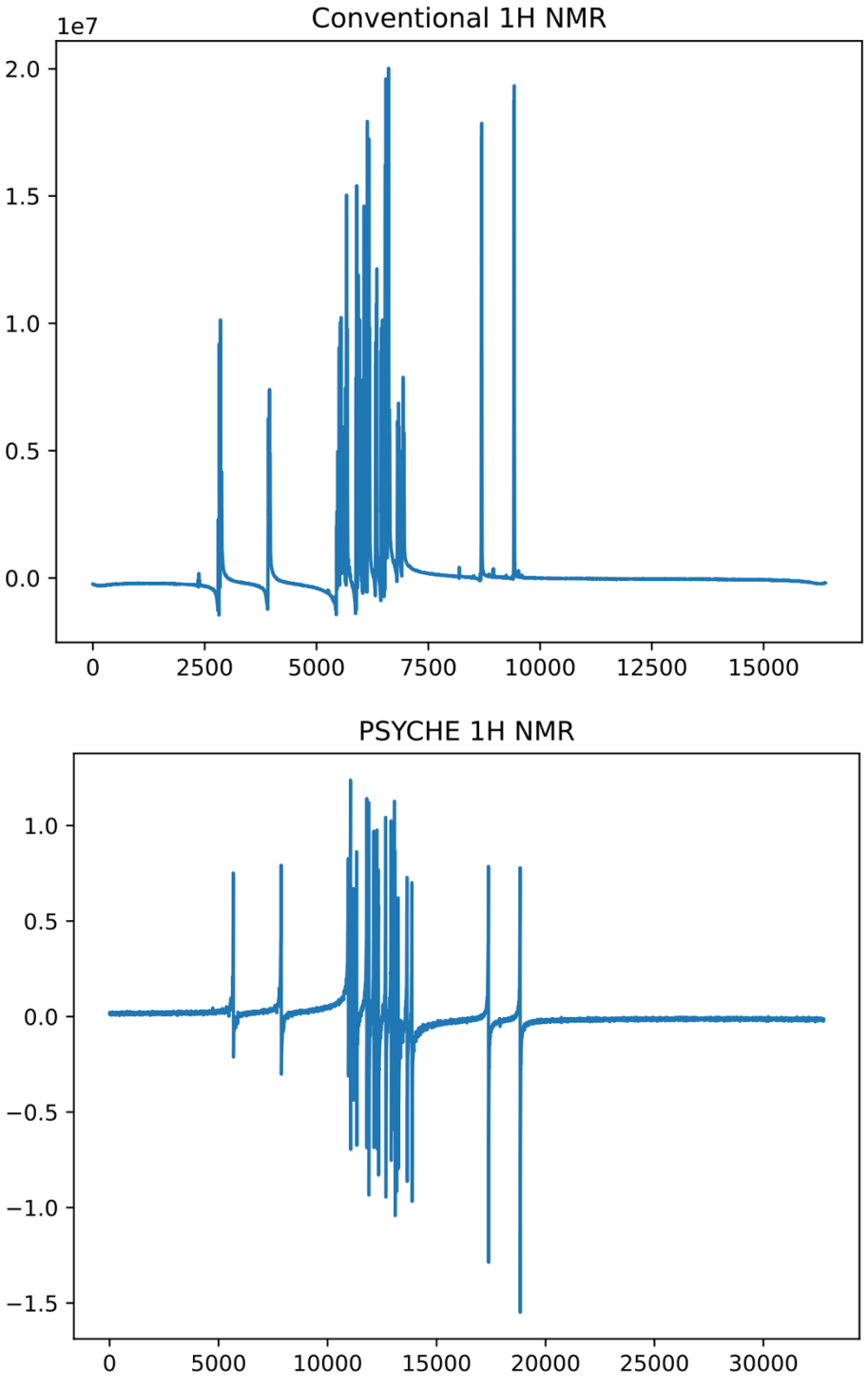




Spectra after resetting phases to zero with --clean_phase 1 and plotted with --phase 1

3. Correct the phases for both spin-echo and psyche with **--phase 1**, and set all of the p0, p1, pp0, and pp1 to the expected values. For example, in this scenario, the initial phase values used are **--p0 -75.0, --p1 270.0, --pp0 50.0, and -pp1 180.0.**

```
python .pureshift \
        --spin_echo 'NMR/Kanamycin/3/' \
        --psyche 'NMR/Kanamycin/1002/' \
        --output 'pred' \
        --phase 1 \
        --p0 -75.0\
        --p1 270.0 \
        --pp0 50.0 \
        --pp1 180.0 \
        --clear_phase 0 \
        --scaling 20 \
        --ver_scale 1.0 \
```

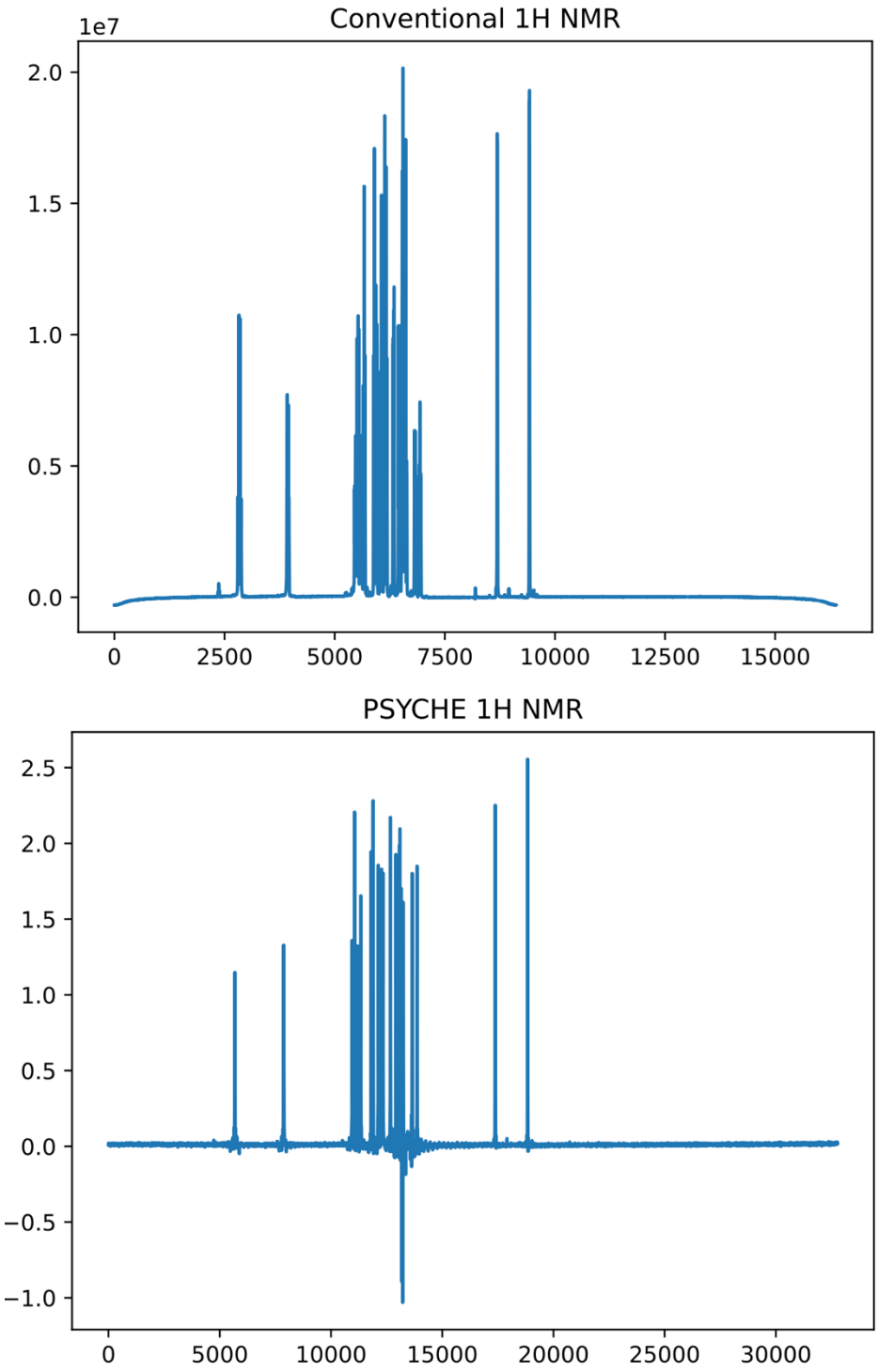


Spectra after the initial step of phase correction with --phase 1

4. Phases to be adjusted further to get proper spectra for both spin-echo and psyche, with **--phase 1**. In this step,
   --p0 –50.0 (total phase is –50.0+(from the previous step –75.0) = –125.0)
   --p1 85.0 (total phase is 85.0+270.0 =355.0)
   --pp0 40.4 (total phase is 40.4+50.0 = 90.4)
   --pp1 115.0 (total phase is 115.0+180.0 = 295.0)

   python .pureshift \
   --spin_echo 'NMR/Kanamycin/3/' \
   --psyche 'NMR/Kanamycin/1002/' \
   --output 'pred' \
   **--phase 1 **
   --p0 -50.0
   **--p1 85.0 **
   **--pp0 40.4 **
   **--pp1 115.0 **
   --clear_phase 0 \
   --scaling 20 \
   --ver_scale 1.0 \

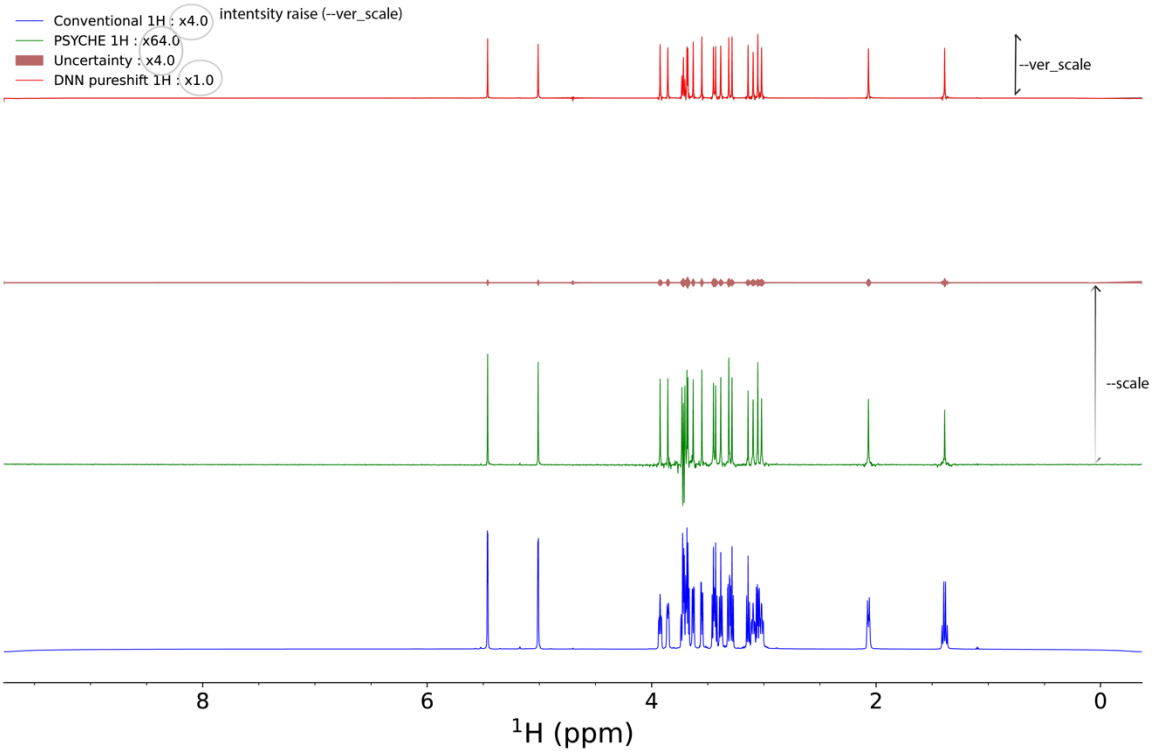
The phase values have now been appropriately set, and this can be seen from the spectra given below. Depending on the requirements, we may need to repeat steps 1–4.



Spectra after full phase correction

5. Once the phase values have been appropriately adjusted, use the argument **--phase 0**, which will execute the **DNN pure shift processing**. The additional parameters, **--scaling** and **--ver_scale** (which can be set at default values), will aid in plotting the spectra with appropriate intensities and spacing between them. Finally, the processed spectra in **.csv** format are saved in the output folder along with a **.pdf** file.

```
python .pureshift \
        --spin_echo 'NMR/Kanamycin/3/' \
        --psyche 'NMR/Kanamycin/1002/' \
        --output 'pred' \
        --phase 0 \
        --p0 0.0\
        --p1 .0 \
        --pp0 0.0 \
        --pp1 0.0 \
        --clear_phase 0 \
        --scaling 20 \
        --ver_scale 1.0 \
```



Final spectra are saved as a PDF file, wherein --ver_scale, and --scale arguments are depicted

How to process only spin-echo spectra while PSYCHE is unavailable

To process only spin-echo spectra with DNN pureshift when PSYCHE is unavailable, delete the --psyche argument, which also applies in the phase correction step.

Phase correction:

```
python .pureshift \
        --spin_echo 'NMR/Kanamycin/3/' \
        --psyche 'NMR/Kanamycin/1002/' \ (delete this line)
        --output 'pred' \
        --phase 1 \
        --p0 0.0\
        --p1 .0 \
        --pp0 0.0 \
        --pp1 0.0 \
        --clear_phase 0 \
        --scaling 20 \
        --ver_scale 1.0 \
```

DNN pureshift processing:

```
python .pureshift \
        --spin_echo 'NMR/Kanamycin/3/' \
        --psyche 'NMR/Kanamycin/1002/' \ (delete this line)
        --output 'pred' \
        --phase 0 \
        --p0 0.0\
        --p1 .0 \
        --pp0 0.0 \
        --pp1 0.0 \
        --clear_phase 0 \
        --scaling 20 \
        --ver_scale 1.0 \
```

How to acquire spin-echo NMR spectra suitable for DNN pure shift processing

Please use the dataset given in the **NMR/Kanamycin/3** along with the **Bruker** compatible pulse sequence **spin-echo_pr** (a presaturation version); however, for the normal cases, where there is no significant water signal, **plw9** can be set to zero.