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1D Batch Processing and SAND Using NMRPipe V.1

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We use this protocol and it's working

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Disclaimer

Abstract

This protocol describes how to batch process and SAND one-dimensional (1D) proton (^{1}H) NMR data.

Before start

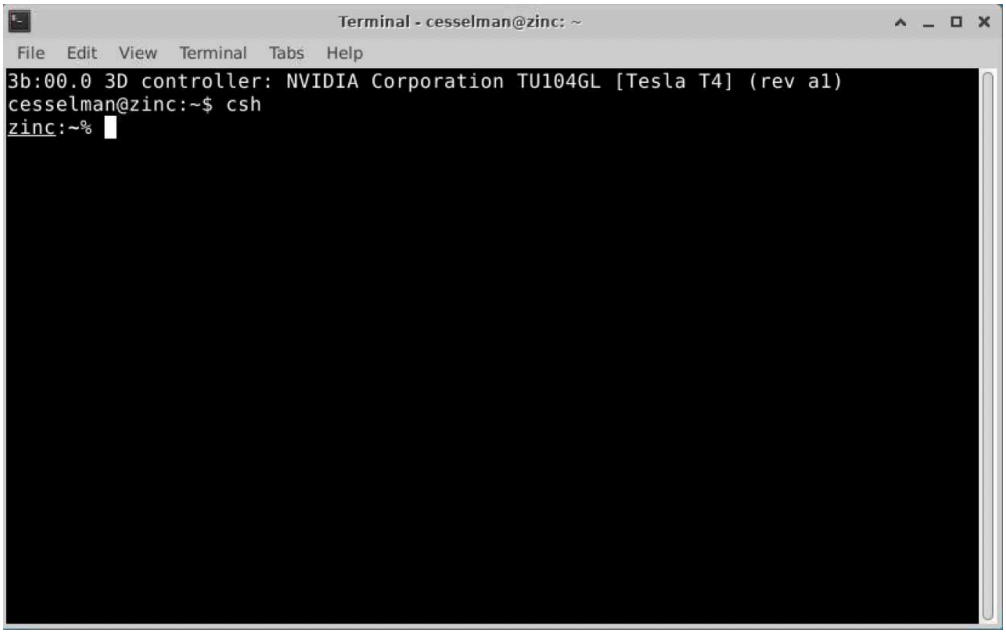
This protocol assumes:

- You have a NMRbox account
- Directions for creating an account can be found at: https://nmrbox.nmrhub.org/pages/getting-started
- This protocol uses NMRPipe. Further Demo Data and processing tips can be found at: https://www.ibbr.umd.edu/nmrpipe/demo.html

Acquire Necessary Scripts

1 Sign in to your NMRbox account.

2 Open the terminal, type csh, and press Enter.



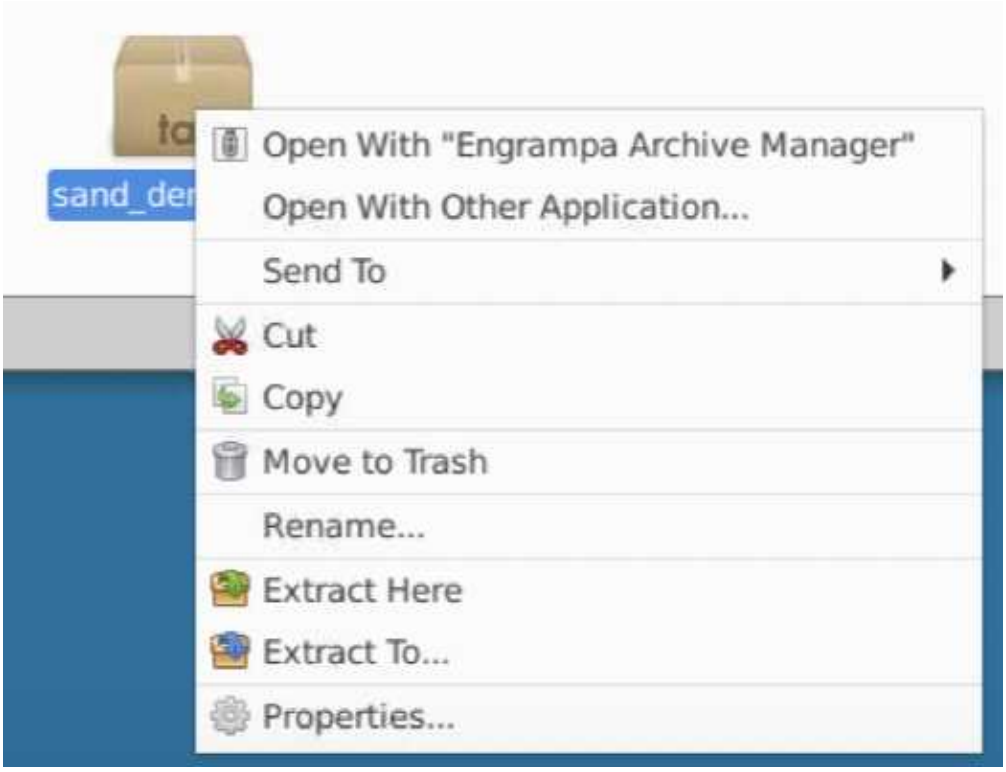
3 Paste the command provided below into the terminal window and press Enter.

Command

Retrieve sand_demo1 files from NMRPipe Website

```
wget https://www.ibbr.umd.edu/nmrpipe/sand_demo1.tar
```

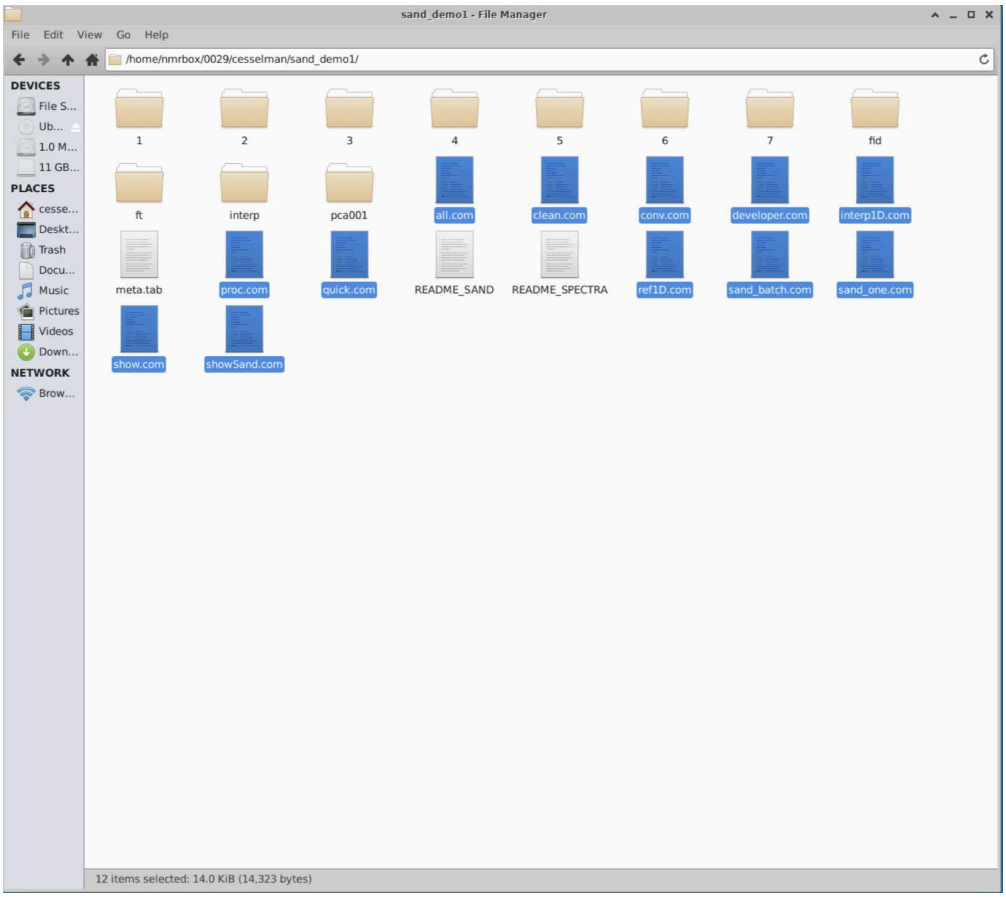
4 Open the File Manager and extract sand_demo1.tar to the home directory by right-clicking on sand_demo1.tar and selecting "Extract Here."



4.1 The contents can also be extracted using the terminal by executing the command below:

```
tar -xvf sand_demo1.tar
```

5 Navigate to the extracted sand_demo1 directory, then copy and paste each ".com" file into the directory that contains your unprocessed data.



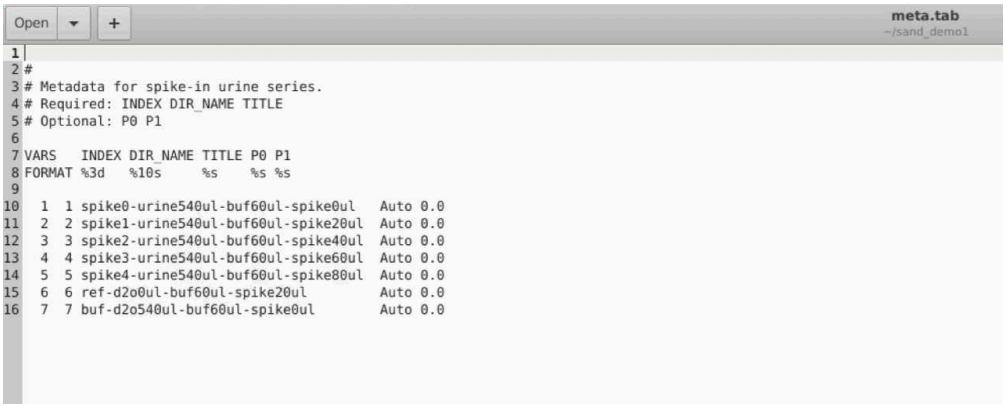
5.1 The ".com" files can also be copied using the terminal:

```
cp ./*.com ~/destination_folder
```

Creating Metadata table

6 Create a copy of meta.tab and place it into the directory containing your unprocessed data.

6.1 Update meta.tab to match the data within your unprocessed directory. Specifically, change the "DIR_NAME" column (the second column of numbers) to match the directories of the spectra you wish to batch process. You should also change the "TITLE" column (the third column) to describe the spectra you are processing, ensuring that there are no spaces in the title name.



6.2 Modifying meta.tab by hand is cumbersome, but you can use the script below to automate the process.

FILE metaTabCreate.sh

1. Place the metaTabCreate.sh script in the same directory as the meta.tab file you just moved.
2. Ensure the file is executable by right-clicking on metaTabCreate.sh, choosing "Properties", selecting
"Permissions," and checking "Allow this file to run as a program".
3. Using a terminal, navigate (cd) to the directory containing the files and enter the command

```
./metaTabCreate.sh
```

4. Provide a title for the dataset, ensuring you do not use spaces in the name.

6.3 Ensure that the rows in the meta.tab file contain metadata only for the files you intend to process. You should delete any rows corresponding to folders that do not contain data or should not be processed.

Perform Processing

7 Using a new terminal window, navigate (cd) into the directory containing the unprocessed data, ".com" files, and meta.tab.

8 Enter the command

```
./all.com
```

The data processing is complete once a graphical image of the spectra appears on the screen. The final processed data will be located in the newly created folder named interp.

9 To view the spectra at any time after processing, open a terminal, navigate to the directory containing the unprocessed and processed data, and enter the command

```
specView.tcl -in interp/*.ft1
```

Optimizing Processing

10 Sometimes, the automatic zero-order phasing does not phase the spectra perfectly. If this is the case, please follow the steps below.

11 Visualize the spectra to identify which spectra are not phased correctly. Then, reprocess the chosen spectra with 0.0 zero-order phasing and 0.0 first-order phasing by changing the "P0" values for those spectra in meta.tab from Auto to 0.0 and then reexecuting

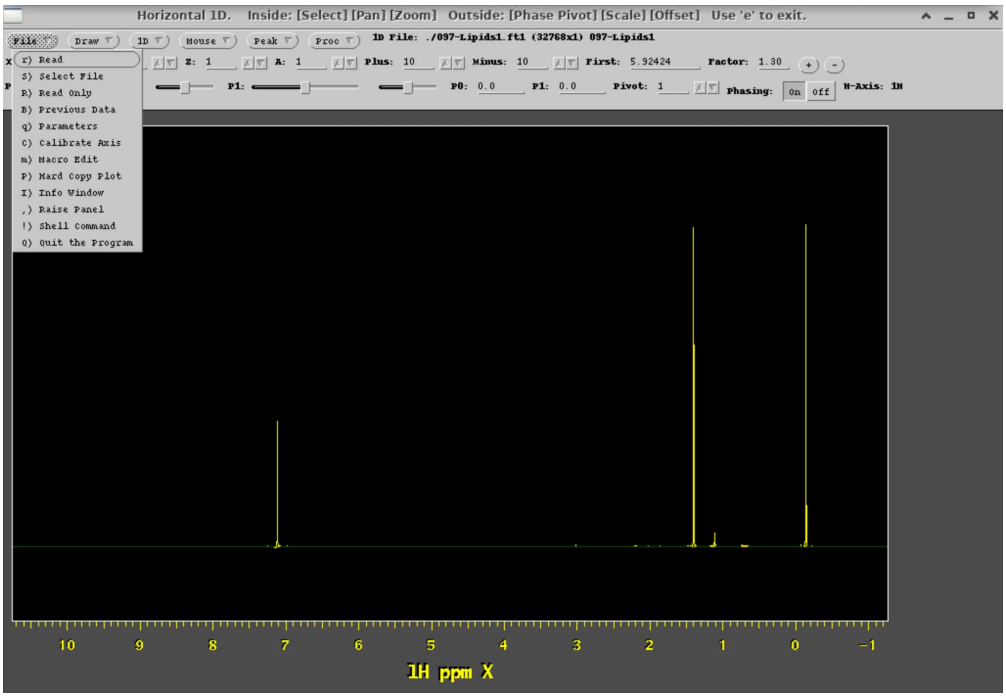
```
./all.com
```

12 After processing is complete, open a new terminal, navigate to the interp folder, and enter the command

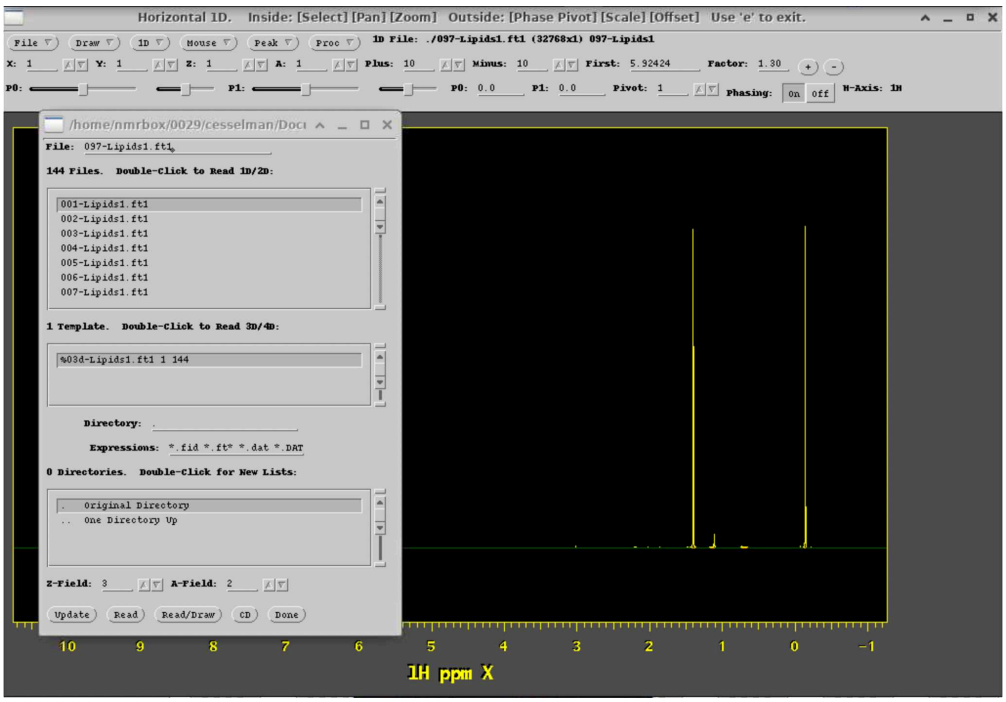
```
nmrDraw
```

Note that nmrDraw functions best when used with a three-button mouse. Further directions on spectral processing and use of NMRPipe can be found at: https://www.ibbr.umd.edu/nmrpipe/index.html

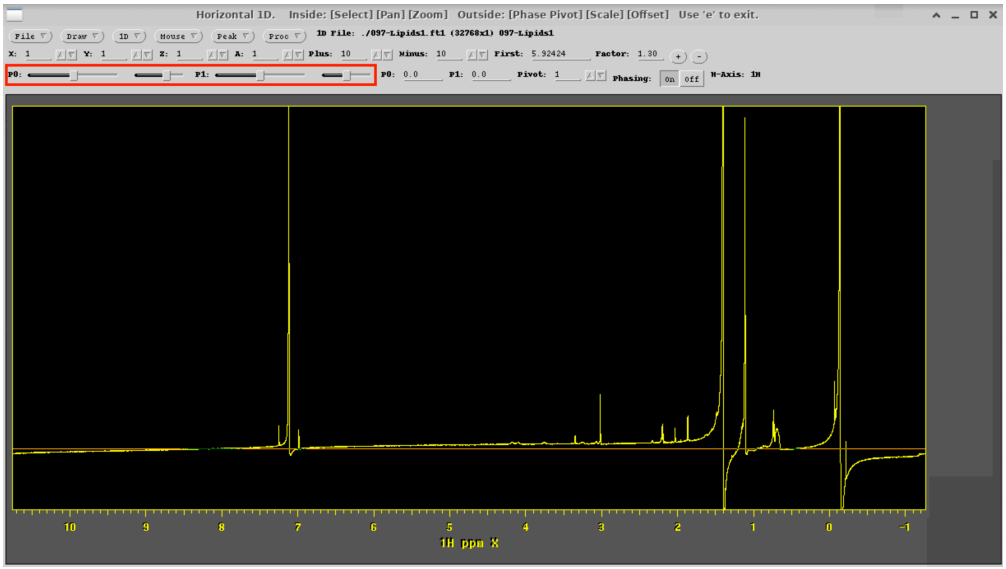
12.1 Select the spectrum you want to phase by first right-clicking on "File" and then left-clicking on "Select File".



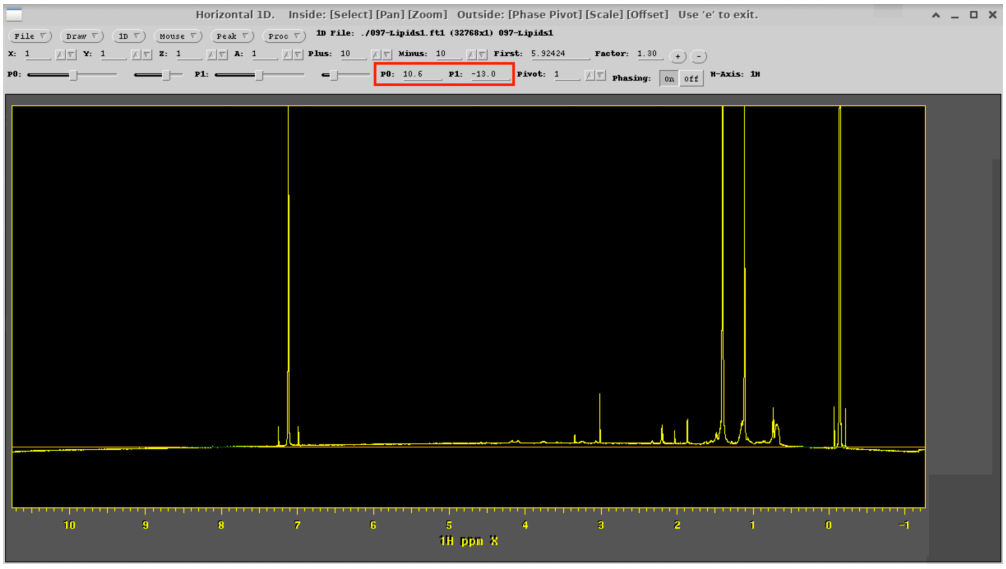
12.2 Use the top sliding bar to scroll through the spectra, and double left-click on the specific spectrum you wish to phase.



12.3 Use the sliders to phase the spectra by left-clicking and dragging them.



12.4 After the phasing looks correct, the values shown in the red box below will be the values used to replace the zero-order and first-order phase values for that spectrum in the meta.tab file.



13 After you have changed the phasing values in the meta.tab file, reexecute

```
./all.com
```

SAND

14 Download the run_sand and copy_csv_sand.sh files from the FLAnalyzer GitHub repository.
https://github.com/edisonomics/FLAnalyzer/tree/main/sand

15 Place the run_sand file into your scratch directory on NMRbox. Your scratch directory is located at the path

```
/scratch/xxxx/username
```

, where xxxx is the number where your NMRbox username is stored (e.g., 0030). You can find this number by opening the terminal on NMRbox and typing

```
pwd
```

; the number appears immediately before your username.

An example output of executing the pwd command is: /home/nmrbox/0030/cesselman
The corresponding scratch folder for this user is: /scratch/0030/cesselman

Some users do not have a number before their name.

An example output of executing the pwd command would be: /home/nmrbox/cesselman
The corresponding scratch folder for this user would be: /scratch/cesselman

15.1 Ensure that the file is executable by using the same method described in Step 6.2.

16 Copy the interp folder created during batch processing into the scratch directory.

17 Edit the run_sand script as follows:

```bash
#!/bin/bash

# Set the source directory on your scratch disk
scratch_directory=""
interp_directory=""

# Set the destination directory on your local machine
local_directory=""

# Define the keyword to search for
keyword="Done"

# Iterate through the files in the source directory
for file in "$interp_directory"/*; do
    if [ -f "$file" ]; then
        # Extract the file name without extension
        filename=$(basename -- "$file")
        filename_noext="${filename%.*}"

         sand1D.com -in "$file" -x1 10ppm -xn -0.5ppm -simAll


        # Copy the resulting folder to the local directory
        mkdir "$local_directory/$filename_noext/"
        cp -r "$scratch_directory/sand0001/"* "$local_directory/$filename_noext/"
        rm -r "$scratch_directory/sand0001"
    fi
done
```

Line 4: Add the path to the scratch directory (e.g., scratch_directory="/scratch/0030/cesselman").

Line 5: Add the path to the interp folder in the scratch directory (e.g., interp_directory="/scratch/0030/cesselman/interp").

Line 8: Add the path to the local folder where SAND results will be saved. Ensure that this local folder already exists.
(e.g., local_directory="/home/nmrbox/0030/cesselman/Documents/").

Line 20: Change the ppm values to cover the full chemical shift range in which peaks appear
(e.g., change 10ppm and -0.5ppm to values that suit your analysis)

Completion: After editing the file, save and close it.

18 On NMRbox, a single user can access up to three Virtual Machines (VMs) simultaneously. To reduce the time needed for SANDing, you should use three VMs. Repeat steps 14 through 17 on the different VMs. In the interp folder for each VM, delete any files that should not be SANDed by that specific VM. For example, if you want to SAND 140 spectra, keep the spectra in the scratch folder as follows: 1-48 on the first VM, 49-96 on the second VM, and 97-140 on the third VM.

19 On each VM, open the terminal, navigate to the scratch directory, and execute

```
./run_sand
```

View SAND Results

20 In the local directory where the SAND results are saved, navigate to the folder of an individual SANDed spectrum. You can use the command below to assess the SAND results.

```
specView.tcl -in ft/*.ft1 sim/0001.ft1 simAll/1/*.ft1
```

Gather SAND CSV Files

21 It is helpful to gather all the SAND tables into a single directory, and this is required for use with FLAnalyzer. Download the copy_csv_sand.sh file from the FLAnalyzer GitHub (Step 14) and ensure the permissions are set to allow the script to run as an executable.

22 Edit the copy_csv_sand.sh script as follows:

```
#!/bin/bash

# Define the output directory where files will be copied
output_dir=""

# Loop through each initial directory
for initial_dir in /Change_to_path_destination_directory/*; do
    if [ -d "$initial_dir" ]; then
        # Get the name of the initial directory
        dir_name=$(basename "$initial_dir")

        # Find the 0001.ft1 file inside each initial directory
        file_to_copy="$initial_dir/csv/0001.csv"

        # Check if the file exists
        if [ -f "$file_to_copy" ]; then
            # Copy the file to the output directory with the desired name
            cp "$file_to_copy" "$output_dir/$dir_name.csv"
            echo "Copied $file_to_copy to $output_dir/$dir_name.csv"
        else
            echo "File $file_to_copy not found."
        fi
    fi
done
```

Line 4: Add the absolute path to the directory where the CSV files will be copied.

Line 7: Change this to the absolute path of the destination directory for the SAND output folders, as specified in Line 8 of the run_sand script (Step 17).

23 Execute the script by entering

```
./copy_csv_sand.sh
```

Protocol references

1. Delaglio, F. et al. NMRPipe: a multidimensional spectral processing system based on UNIX pipes. *J. Biomol. NMR*. **6**, 277-293 (1995).

2. Wu, Y. et al. SAND: Automated Time-Domain Modeling of NMR Spectra Applied to Metabolite Quantification. *Anal Chem* **96**, 1843-1851 (2024).

Acknowledgements

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