Supplementary Material

Workflow for Data Analysis in Experimental and Computational Systems Biology: Using Python as 'Glue'

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Instructions for Running Supplementary Jupyter Notebooks

The file `ArchiveS2_Supplementary_notebooks.zip` contains four folders with Jupyter notebooks and associated data to recreate the analyses that are presented in the main paper. To execute these notebooks, you will need to set up two different Python 3 virtual environments. The easiest way to set up a system with the prerequisites if you do not yet have a Python 3 installation, is to install the Anaconda Software Distribution (https://www.anaconda.com/distribution), which is freely available for Windows, macOS and Linux. But an existing Python 3 installation can also be used.

The following notebook needs to be executed in the `nmrpy` environment:

- NMR_processing_tutorial (recreates Figure 2 in main paper)

The following notebooks need to be executed in the `pysces` environment:

- Plate_assay_fitting_tutorial (recreates Figure 3 in main paper)
- NMR_fitting_tutorial (recreates Figure 4 in main paper)
- Validation_tutorial (recreates Figure 5 in main paper)

Two different virtual environments are needed because the version of `matplotlib` required by `nmrpy` is different from the version required by the other packages.

Virtual environment for NMRPy

Create and activate virtual environment named `nmrpy`, ensure that the Python interpreter is version 3.6 or 3.7. If you have `virtualenvwrapper` installed, this is easily done with:

```
mkvirtualenv -p path/to/my/python3interpreter nmrpy
```

Anaconda has its own syntax for creating virtual environments:

```
conda create -n nmrpy python=3.7
```

Once the virtual environment is activated, as shown by the "`(nmrpy) $`" or similar prompt, install the required packages with:

```
(nmrpy) $ pip install git+https://github.com/jmrohwer/nmrpy
(nmrpy) $ pip install notebook
```

Once you have started the Jupyter notebook server inside this virtual environment, you should be able to run the NMR_processing_tutorial notebook.

Virtual environment for PySCeS

Create a second virtual environment named `pysces`, also with Python version 3.6 or 3.7, using the same method as above. Activate the virtual environment and install the required packages:

```
(pysces) $ pip install pysces
(pysces) $ pip install notebook
(pysces) $ pip install ipympl
(pysces) $ pip install ipywidgets
(pysces) $ pip install lmfit
(pysces) $ pip install pandas
(pysces) $ jupyter nbextension enable --py widgetsnbextension --sys-prefix
```

Once you have started the Jupyter notebook server inside this virtual environment, you should be able to run the other notebooks:

- Plate_assay_fitting_tutorial
- NMR_fitting_tutorial
- Validation_tutorial