
Frazier-PipeLine Documentation

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Henry Herbol

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Contents:

FRAZIER PIPELINE

Pipeline for submitting solubility simulations. Bonus output may include Unsaturated Mayer Bond Order amongst other things.

1.1 Installing

Currently installation involves first installing clancelot:

```
cd ~; git clone git@github.com:clancylab/clancelot2.0.git
```

And then cloning this project:

```
cd ~; git clone git@github.com:hherbol/frazier-pipeline.git
```

Note, you'll also have to append the frazier-pipeline/pys folder to your PYTHONPATH variable.

```
echo 'export PYTHONPATH="/PATH/TO/FRAZIER/PIPELINE/pys:$PYTHONPATH"' >> ~/.zshrc
```

1.2 Documentation

Documentation is necessary, and the following steps MUST be followed during contribution of new code:

Setup

1. Download [Sphinx](#). This can be done simply if you have [pip](#) installed via `pip install -U Sphinx`
2. Wherever you have *frazier-pipeline* installed, you want another folder called *frazier-pipeline-docs* (NOT as a subfolder of frazier-pipeline).

```
cd ~; mkdir frazier-pipeline-docs; cd frazier-pipeline-docs; git clone -b gh-pages  
git@github.com:hherbol/frazier-pipeline.git html
```

3. Forever more just ignore that directory (don't delete it though)

Adding Documentation

Documentation is done using [ReStructuredText](#) format docstrings, the [Sphinx](#) python package, and indices with autodoc extensions. To add more documentation, first add the file to be included in *docs/source/conf.py* under *os.path.abspath('example/dir/to/script.py')*. Secondly, ensure that you have proper docstrings in the python file, and finally run *make full* to re-generate the documentation and commit it to your local branch, as well as the git *gh-pages* branch.

For anymore information on documentation, the tutorial follwed can be found [here](#).

1.3 Using FPL

INDICES AND TABLES

- `genindex`
- `modindex`
- `search`