**Installation:**

1. Create a conda environment created from the requirements file environment.yaml

2. Clone PyMuDRA (https://github.com/MikolajMizera/pyMuDRA) and update its filepath in models.py

3. Construct models by running python train\_models.py. Models will be saved to the folder models, which will be created if it doesn’t already exists

4. Run models on external molecules following the example file run\_models.py

**Notes:**

Exact model files used in the paper are not provided here, but these are exact model architectures and training procedures. Validation statistics produced with this code should be very similar to what is reported in the paper.