

ProteinMPNN (latest code on Oct 25, 2023)

Webpage

<https://github.com/dauparas/ProteinMPNN>

Version

latest code on Oct 25, 2023

Installation

ProteinMPNN

```
$ git clone https://github.com/dauparas/ProteinMPNN.git 20231025
```

python env (miniforge)

```
$ sh Miniforge3-Linux-x86_64.sh
...
[...] >>> /apl/ProteinMPNN/20231025/miniforge3
...
$ ./miniforge3/bin/conda shell.csh hook > conda_init.csh
$ ./miniforge3/bin/conda shell.bash hook > conda_init.sh
$ . conda_init.sh
$ conda install cudatoolkit=11.7.1 pytorch==1.13.1 torchvision==0.14.1 torchaudio==0.13.1 pytorch-cuda=11.7 -c pytorch -c nvidia
```

Mar 27, 2024: additional package for LigandMPNN

```
$ conda install prody pyparsing==3.1.1
```

Notes

- please see notes of [RFdiffusion](#).
- LigandMPNN has problem with pyparsing 3.1.2
 - <https://github.com/dauparas/LigandMPNN/issues/11>