1. Hardware:

* CPU : 8 cores
* Memory: 64 GB
* GPU: 1 Titan V

2. Software:

* CUDA 10.0 CuDNN 7.4
* Anaconda Python 3.7 2019.03
* pytorch==1.1.0
* pytorch\_geometric
* openbabel
* torch\_contrib

3. Re-run Training:

* Run all notebooks in 3 folders: guillaume, thanhtu, lam following corresponding README inside each folder
* Run the stacking\_final notebook
* Estimated time: ~ 600h for training