**Environment Requirements:**

Please refer to the GitHub page: <https://github.com/chen709847237/SSL-GCN>

**Prediction Command:**

python main.py

-d <input data path>

-m <model folder path>

-t <endpoint selection {'NR-AR', 'NR-AR-LBD', 'NR-AhR', 'NR-Aromatase', 'NR-ER', 'NR-ER-LBD', 'NR-PPAR-gamma', 'SR-ARE', 'SR-ATAD5', 'SR-HSE', 'SR-MMP', 'SR-p53'}>

-o <output folder path>

e.g.

python main.py -d ./test\_data.fst -m ./model/ -t NR-AR -o ./test/

**Input data example:**

File **test\_data.fst**, FASTA-like format.

>TEST0

A1222()\*&^%2333ANCNDBSNXBDC

>TOX3753

O=C1Cc2cc(CCN3CCN(c4nsc5ccccc45)CC3)c(Cl)cc2N1

>TEST1

A12222333ANCND\*&^%BSNXBDC()

**Output result example:**

File **test\_data\_result.csv**

**表格

描述已自动生成**

0 represents non-toxic

1 represents toxic

If the entered SMILES string is incorrect or cannot be converted to a graph, "invalid mol" will be given as its result.