Tutorial of KokumiPD

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1. Offline version deployment

1.1 Installation of python dependencies

numpy 1.24.3
rdkit 2023.3.2
torch 2.0.1+cpu
dgl 1.1.1
dglife 0.3.2

1.2 Run KokumiPD

python predictor.py
-h, --help show this help message and exit
-t {0,1}, --type {0,1}
0 is Graph Neural Network (GNN) for predict kukumi/non-kokumi,
1 is Support Vector Machine (SVM) with 2D-fingerprint RDKFP as input
-i FILE, --file FILE input smiles file, don't have a header, only a column smiles
-o OUT, --out OUT output file

2. Webserver version deployment

2.1 MySQL

Dowaload and install from https://www.mysql.com/
$ mysql -u username - p password
> create database kokumi;

2.2 Django

Dowaload and install from https://www.djangoproject.com/
Installation of python dependencies
$ pip install djangorestframework
$ pip install django-cors-headers
Configuring the database information in settings.py
Configuring the cross-domain information in settings.py
$ python manage.py migrate
$ python manage.py makemigrations
$ python manage.py migrate
$ python manage.py runserver

2.3 Vue

Dowaload and install from https://cn.vuejs.org/
Configure your backend API
$ npm run dev