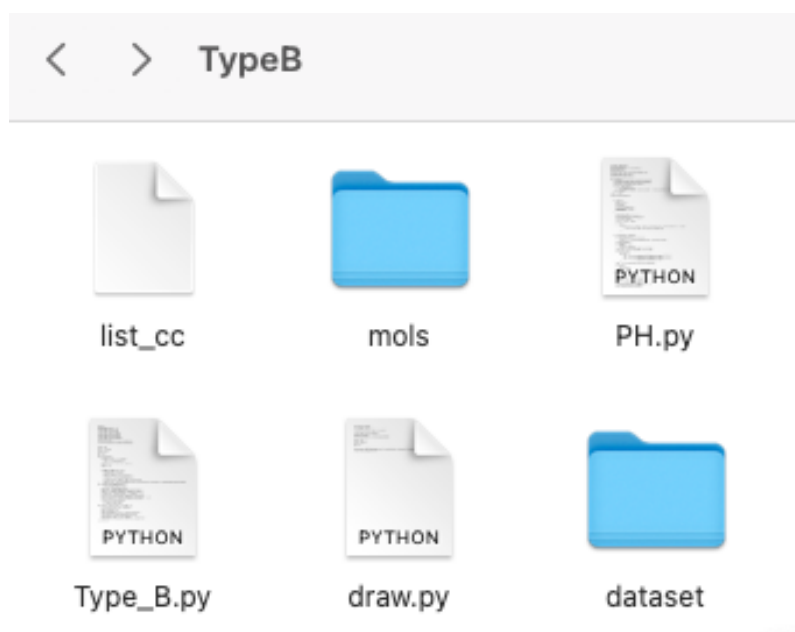


## README file for Type B



1. list\_cc : the dataset from paper “Computational Predictions of Glass-Forming Ability and Crystallization Tendency of Drug Molecules”.
2. mols: the conformation files of each molecule in the dataset are stored in XYZ format.
3. PH.py: the relevant algorithms for persistent homology.
4. Type\_B.py: the code to generate the feature matrix using Type B descriptors.

```
Type_B.py x
10 import collections
11 from sklearn.preprocessing import MinMaxScaler
12
13 collections.Iterable = collections.abc.Iterable
14
15 pixel_m = 40
16 pixel_n = pixel_m
17
18 sigma = 0.015
19 Max = 2.5
20 Min = -0.1
21
22 def build_dataset():
```

The table below shows the correspondence between the variables in the code and those in the article.

Variables in the code	Variables in the article
pixel_m	$\mathfrak{M}$
pixel_n	$\mathfrak{N}$
Max	maxBD
Min	minBD
sigma	$\sigma$

You can modify “sigma” ( $\sigma$ ) to obtain descriptors with different Gaussian kernel.

5. draw.py: the demonstration of Persistence Image (PI).

6. dataset: the feature matrices corresponding to different values of  $\sigma$  are used for model selection.