a.

1

PubChem, ZINC, HMDB, etc.

Data filter

ab initio calculation

qcMol Dataset

Refresh   Calculate

Search

2

Loss

Global Token

Structure Features

Atom Features

Bond Features

Preprocess

Encoder

Stacked by *N* Layers Encoding blocks

< 0.98, 0.8, 2.9, ... >
< ..., ..., ... >
< 0.99, 0.07,...,0.20 >
< 0.20, 0.33,..., 7.00 >

Decoder

Information Recovery

3

Downstream Application

ADMET Prediction

Protein Ligand Interaction

Compound Generation

Other tasks