Tutorial of fragment split by MolAICal

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1. Introduction

Sometime, to study the fragment properties of ligands, the ligands need to be split into smaller pieces. Here, MolAlCal provides a way to split ligands into small fragments according to rotatable bonds. In this tutorial, the method of fragment split is introduced based on the protocol of MolAICal (https://doi.org/10.1093/bib/bbaa161).

2. Materials

2.1. Software requirement

1) MolAICal: https://molaical.github.io

2.2. Example files

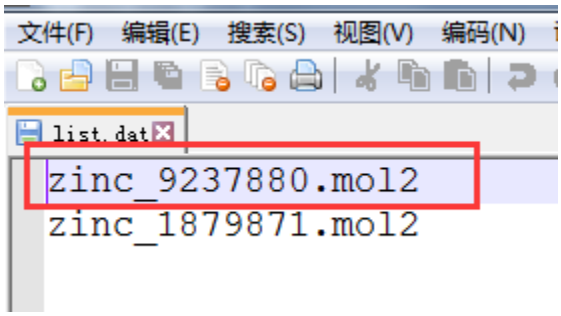
1) All the necessary tutorial files are downloaded from:
https://github.com/MolAICal/tutorials/tree/master/013-fragmentSplit

3. Procedure

Change directory to "013-fragmentSplit":

#> cd 013-fragmentSplit

Preparing the input file named "list.dat" that contains the files' name of ligands:



1. Split ligands into small fragments without adding or deleting hydrogen

#> molaical.exe -tool fragSplit -i list.dat -o inital -oa results

Or

#> molaical.exe -tool fragSplit -i list.dat -o inital -oa results -w off

2. Split ligands into small fragments with adding hydrogen

#> molaical.exe -tool fragSplit -i list.dat -o inital -oa results -w add

3. Split ligands into small fragments with deleting hydrogen

#> molaical.exe -tool fragSplit -i list.dat -o inital -oa results -w del

Note: The folder "initial" includes split fragments without adding or deleting hydrogen. The folder "results" contains fragments that have been dealt with command parameter "-w". The parameter "-w" indicates whether MolAICal deletes or adds hydrogens on the receptor.

If you want to merge the split fragments or ligands into one file, the command can be used as below:

```
#> molaical.exe -tool merge -m mol2 -i results -o all_frag.mol2
```