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.

2. Materials

2.1. Software requirement

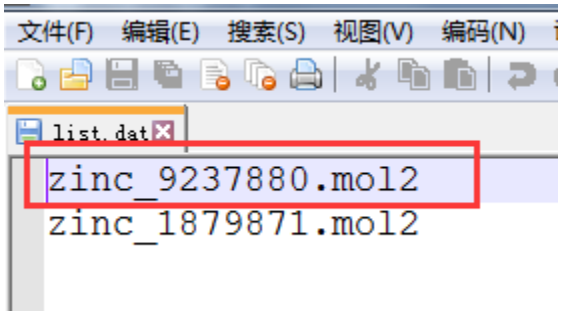
1) MolAICal: https://molaical.github.io

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