Script Path: /home/cai/python\_script

1. Import fort.38 occupancies into head3.lst, excluding the cluster residues.

Input file: head3.lst, fort.38, ms\_gold(cluster residues)

Script: update\_adv.py

Run: ./update\_adv.py fort.38 head3.lst ms\_gold

1. Run MCCE step4. Enumeration.

Input file: ms\_gold (cluster residues),

Parameter: run.prm: 10000 Maximum microstates for analytical solution (NSTATE\_MAX)

0.000 Cut-off occupancy of the reduction (MONTE\_REDUCE)

t Output Microstate (MS\_OUT)

t Output readable micristate file from standard monte carlo (RE\_MS\_OUT)

Run: /home/cai/mcce3.5\_enum\_ms/mcce.

1. Post analysis: aggregate same ionization states or microstates together.

Input file: ms.dat or re\_ms.dat

Script: mfe\_adv.py, ms\_cor\_new.py

Run: python ms\_cor\_new.py