MCCE runs:

1. Run with free titration for all A+B, get fort.38, head3.lst.ori
2. Head3.lst: fix B in PB distribution. A is free to titrated.

Eg: /archive/cai/ba3/xray/quick\_run\_mdlip/step4/enum\_E/3s8f

A residue list should ms\_god

At ../: /home/cai/python\_script/update\_adv.py fort.38 head3.lst.ori ms\_gold > head3.lst

1. Rerun step 4 with microstate output:

Run.prm: (NSTATE\_MAX) increase the limit if necessary.

Post analysis:

1. Output all ionization states of A and their detailed energy terms of microstate with minimum energy.

Cmd: /home/cai/python\_script/ public\_script/ms\_agg.py sheetname

Ms\_agg.py needs mfe\_adv.py and energy\_adv2.py

Parameter setting:

Outputfile setting in ms\_agg.py: outputfile='./ms\_E.xlsx'

1. Output most occupied microstate of A with occupancy >0.1

Cmd: /home/cai/python\_script/ public\_script/ms\_occ.py sheetname

Parameter setting:

Outputfile setting in ms\_agg.py: outputfile='./ms\_occ.xlsx'

Uncomment write\_ms\_occ(outputfile, sheetname)

1. Output all microstates’ energy value within 3kcal range.

Cmd: /home/cai/python\_script/ public\_script/ms\_occ.py sheetname

Outputfile setting in ms\_agg.py: outputfile='./ms\_crgseq.xlsx'

Uncomment write\_ms\_crgseqs(outputfile, sheetname)