The new formats of MS will be a folder named ms\_out creating to store each titration point microstates. And the file name is ph#eh#ms.dat.

The file format will be:

1st line: contain constant information, Temperature, ph, eh,

2nd line: method: MONTERUNS or ENUMERATE.

3rd line: fixed residues number: fixed conformer id with occupancy > 0.99 (considering that conformer that are partially occupied).

For MONTERUNS:

Because each MC cycle starts from a new microstate, so the free residue conformer id needs to be remember for each cycle.

4th line: MC cycle number

5th  line: free residue number: free conformer id for the starting microstate, it may or may not be accepted later.

6th line: flips, state energy, count

For ENUMERATE:

4rd line: free residue number: free conformer id

5th line: flips, state energy, occ

Here are the examples:

MONTERUNS

T:298.15,pH:  7.00, eH:  0.00

METHOD: MONTERUNS

#N\_FIXED: FIXED\_CONF\_ID,

33: 4, 5, 17, 18, 19, 20, 35, 93, 94, 104, 105, 111, 128, 129, 138, 145, 157, 158, 176, 217, 232, 239, (the number of conf here <= n\_fixed)

#EVERY MONTERUN START FROM A NEW STATE

#ITER\_MONTERUNS

#N\_FREE: FREE\_CONF\_ID,

#FLIPS, ENERGY, COUNT

MC: 0

43: 0, 7, 28, 30, 48, 53… (the number of conf here == n\_free)

-86.736252, 3

731, -86.540253, 2

221, -86.407249, 18

60, -87.149246, 1

146, -86.984253, 1

ENUMERATE

T:298.15,pH:  7.00, eH:  0.00

METHOD: ENUMERATE

#N\_FIXED: FIXED\_CONF\_ID,

689: 4, 19, 21, 22, 28, 29, 33, 43, 45… (the number of conf here <= n\_fixed)

#N\_FREE: FREE\_CONF\_ID,

#FLIPS, ENERGY, OCC

6: 487, 674, 689, 1286, 1487, 1495, (the number of conf here == n\_free)

522.549866, 0.000

488, 525.786072, 0.000

489, 523.460388, 0.000

490, 522.563965, 0.000

FLOW CHART TO CREATE MICROSTATE OUTPUT

1. MSRECORD: conf\_id; H; counter; occ; Hav; # for old format ms.dat

conf\_flip\_id; n\_flip; # for new format ms.dat

1. ms\_fp\_test: ms.dat binary file (old format)

ms\_fp: ms.dat txt file (old format)

ms\_fp2: ms.dat (new format)

1. new\_ms\_flag: flag to trigger on or off new format ms.dat output.
2. Load\_ms\_gold: load special residue list for old format ms.dat, using to output microstates of the special residue in ms\_gold.

Main flow chart: monte()

For i == titr\_step

If env.ms\_out ==1?

Load\_ms\_gold: load ms\_spe\_lst

Mkdir MS\_DIR: store new ms.dat at each pH

Open ms\_fp2 in MS\_DIR: new ms.dat

Write T, pH, eH

write ms\_spe\_lst in ms\_fp\_test/ms\_fp ms

Old ms.dat new ms.dat (if new\_ms\_flag=1)

new ms.dat (if new\_ms\_flag=1)

Enumerate\_new==-1?

Write Method, fixed\_conf\_id

Write Method

For j == monte\_run

Write MC: j

MC\_smp(N\_smp): output ms.dat

MC(N\_smp): not output ms.dat

Close ms\_fp/ms\_fp\_test

Close ms\_fp2

Env.ms\_out==0

Old ms.dat new ms.dat (if new\_ms\_flag=1)

flow chart: MC\_smp(N\_smp)

While iters

Initialize ms\_state/old\_ms\_state: MSRECORD struc

Write beginning testing microstate

Memcpy ms\_state to old\_ms\_state

Save flips/n\_flip in ms\_state.conf\_flip\_id/n\_flip

Make flips

Accept?

Write\_ms: write out ms\_state

Update\_conf\_id: update ms\_state.conf\_id

Write\_state\_MC (old\_ms\_state):

Write out old\_ms\_state

Memcpy old\_ms\_state to ms\_state

ms\_state.counter += 1

Write\_ms: write out ms\_state

Write out final ms\_state

Write\_state\_MC (ms\_state):

Write out final ms\_state

No

new ms.dat (if new\_ms\_flag=1)

flow chart: enumerate\_new()

Write\_state\_Enum(&ms\_state)

While iters

Initialize ms\_state: MSRECORD struc

Write beginning microtate: fixed\_conf\_id/free\_conf\_id;

Write\_state\_Enum(ms\_state).

Save flips/n\_flip in ms\_state.conf\_flip\_id/n\_flip

Make flips

Write\_ms(&ms\_state):

write first microtate

If env.ms\_out==1

Update\_conf\_id:

Ms\_state.conf\_id

Write\_ms(&ms\_state):

write each microtate

new ms.dat (if new\_ms\_flag=1)