

Upper limit CCS value: 208.823

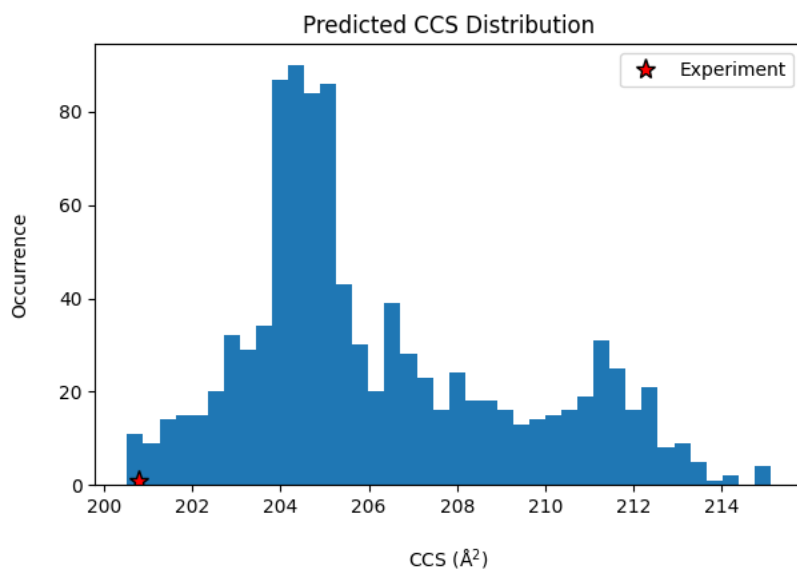
Lower limit CCS value: 192.717

ML Prediction Statistics:

CCS Values
count 1000.000000
mean 206.217682
std 3.121148
min 200.525467
25% 204.103638
50% 205.121429
75% 208.189182
max 215.108566

Completed run remark:

¶ Captured 780 conformers out of a total 1000 conformers
¶ Captured conformers have been siphoned off to Completed_Job/Flavin-mononucleotide/conformer/opt-Flavin-mononucleotide_Rank1_focus_CCS_200.77



Upper limit CCS value: 208.823

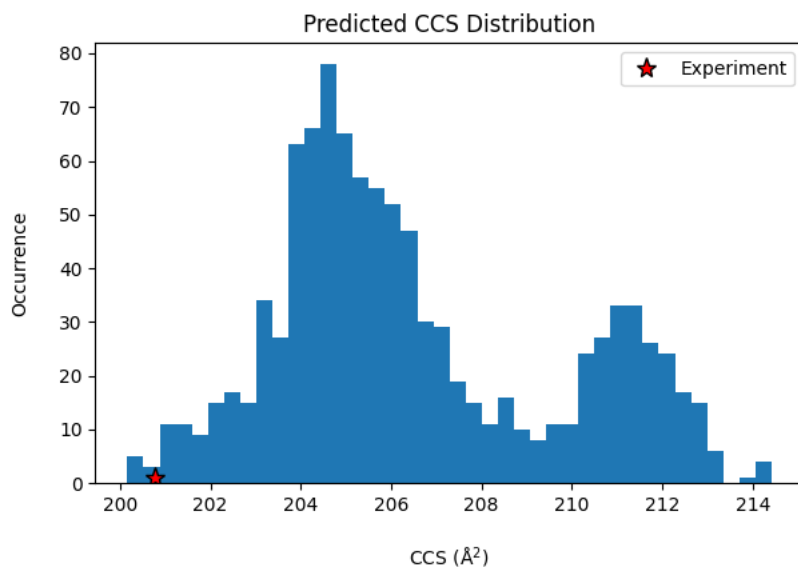
Lower limit CCS value: 192.717

ML Prediction Statistics:

CCS Values
count 1000.000000
mean 206.506638
std 3.139738
min 200.166046
25% 204.287914
50% 205.641510
75% 208.664963
max 214.418289

Completed run remark:

¶ Captured 754 conformers out of a total 1000 conformers
¶ Captured conformers have been siphoned off to Completed_Job/Flavin-mononucleotide/conformer/opt-Flavin-mononucleotide_Rank2_focus_CCS_200.77



Upper limit CCS value: 208.823

Lower limit CCS value: 192.717

ML Prediction Statistics:

CCS Values
count 1000.000000
mean 206.669037
std 3.090377
min 200.343826
25% 204.450031
50% 205.940460
75% 208.698437
max 214.636307

Completed run remark:

¶ Captured 760 conformers out of a total 1000 conformers
¶ Captured conformers have been siphoned off to Completed_Job/Flavin-mononucleotide/conformer/opt-Flavin-mononucleotide_Rank3_focus_CCS_200.77

