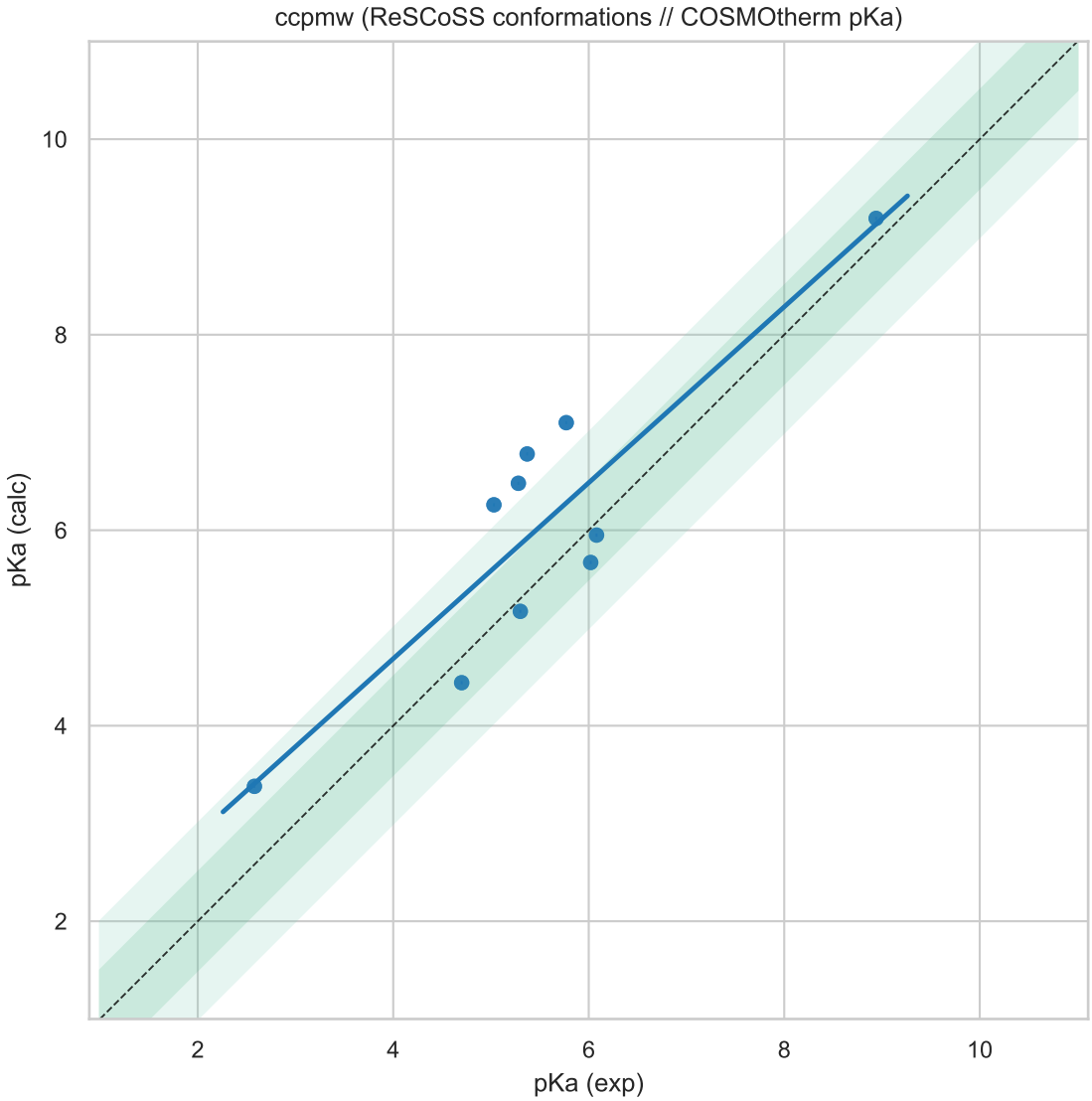
ccpmw (ReSCoSS conformations // COSMOtherm pKa)
pKa (calc)
pKa (exp)
2
4
6
8
10