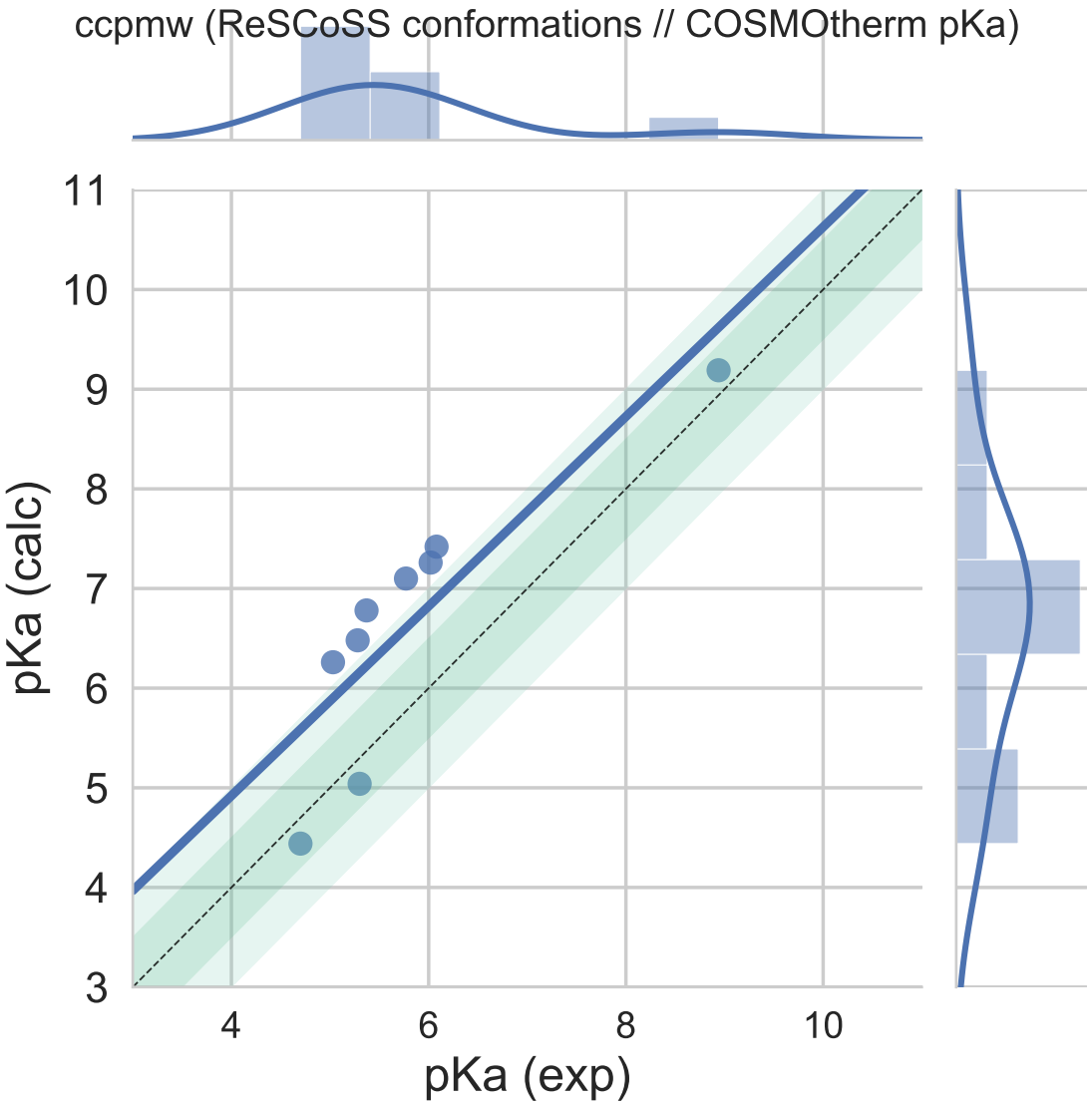
ccpmw (ReSCoSS conformations // COSMOtherm pKa)
pKa (calc)
pKa (exp)
11
10
9
8
7
6
5
4
3
4
6
8
10