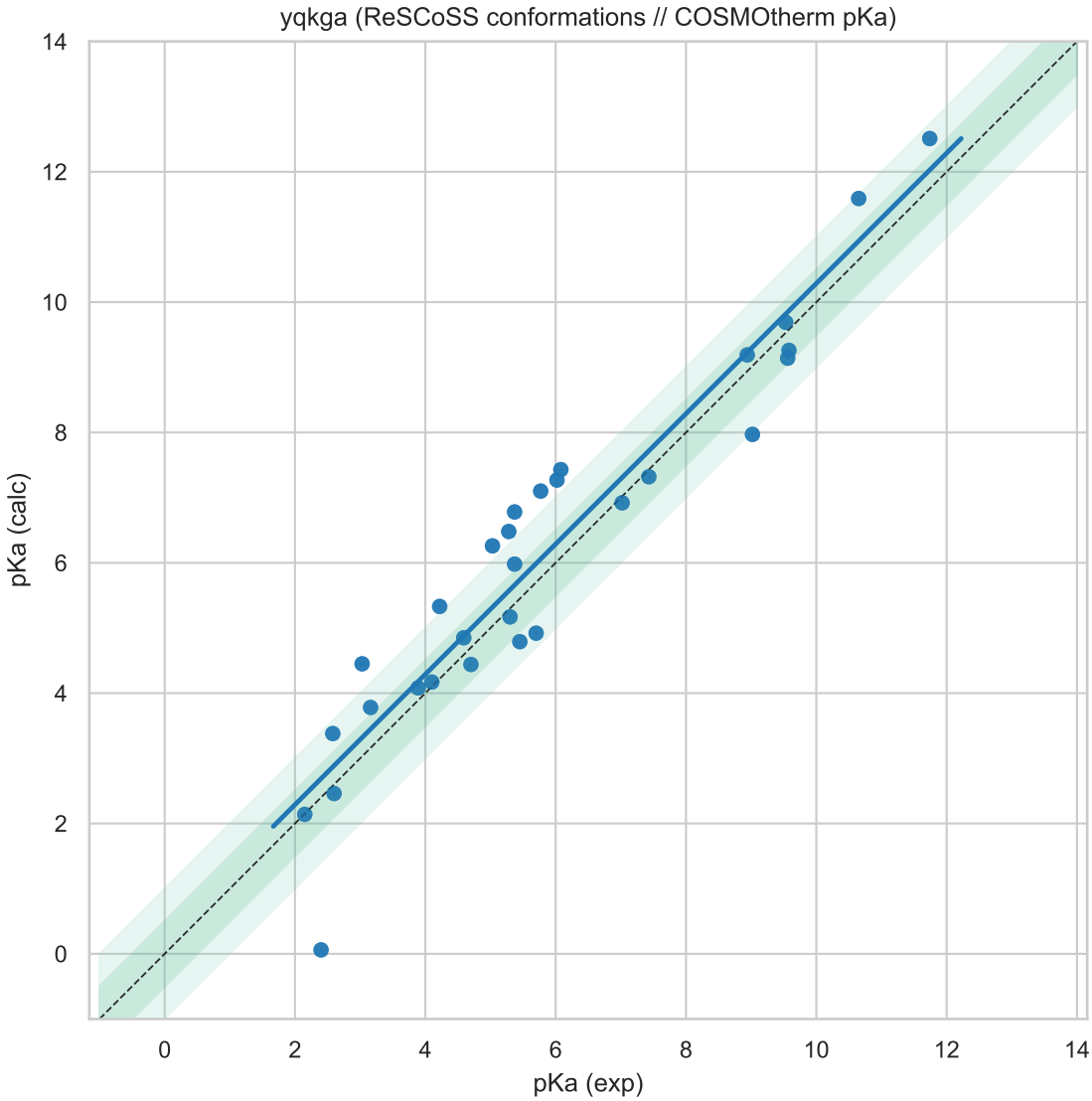
yqkga (ReSCoSS conformations // COSMOtherm pKa)
pKa (calc)
pKa (exp)
14
12
10
8
6
4
2
0
0
2
4
6
8
10
12
14