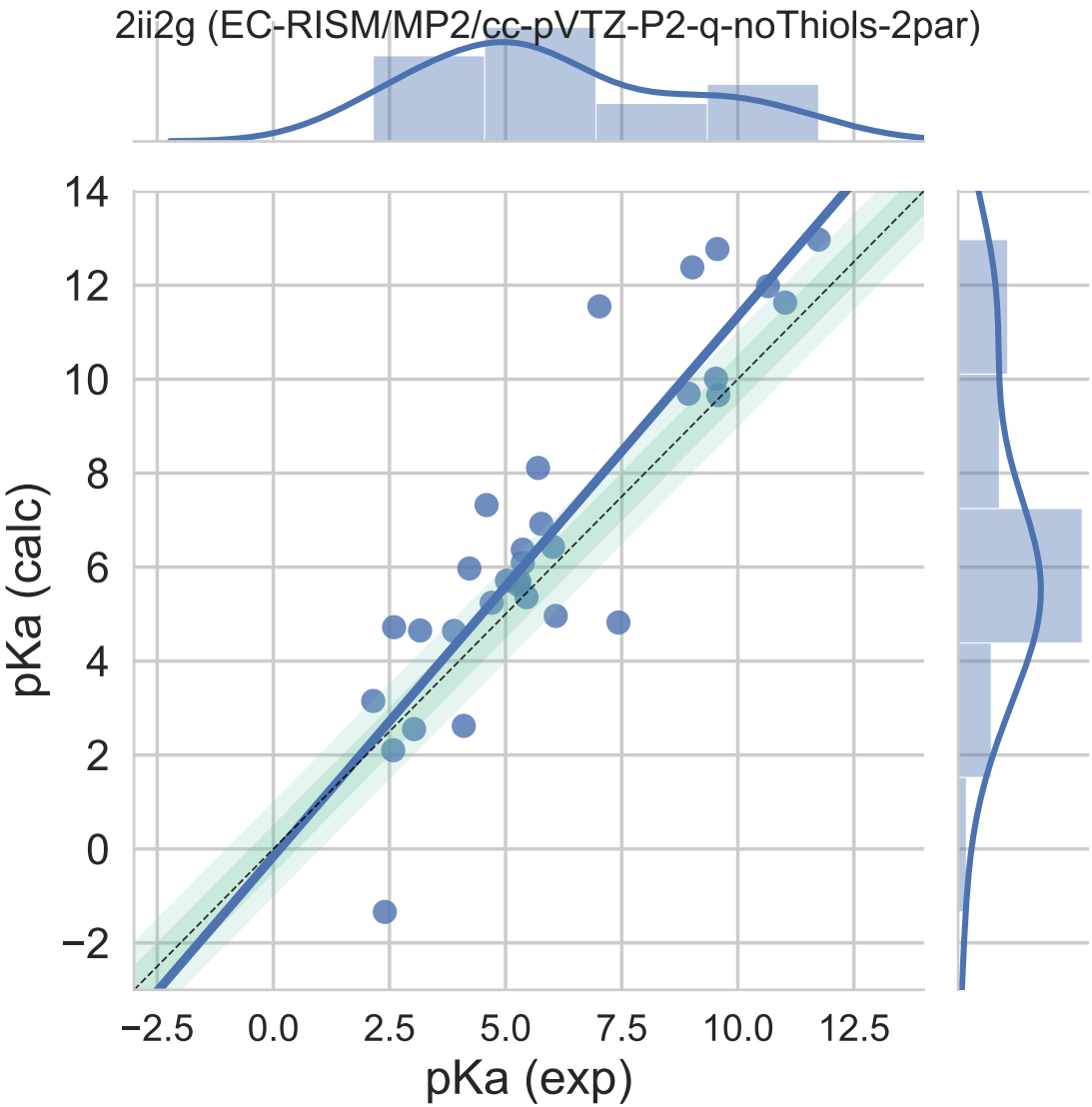
2ii2g (EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par)
pKa (calc)
pKa (exp)
14
12
10
8
6
4
2
0
−2
−2.5
0.0
2.5
5.0
7.5
10.0
12.5