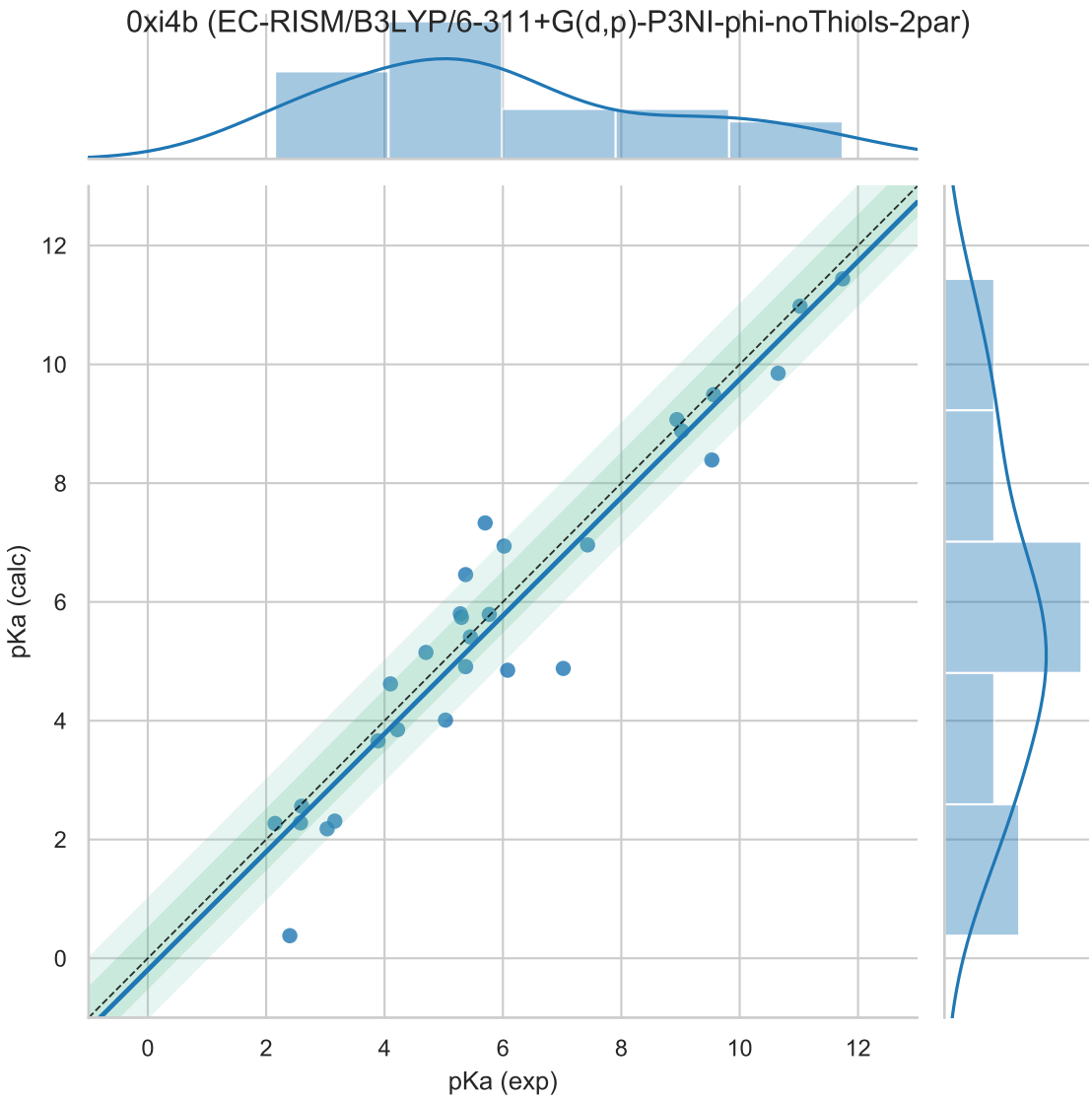
0xi4b (EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par)
pKa (calc)
pKa (exp)
0
2
4
6
8
10
12