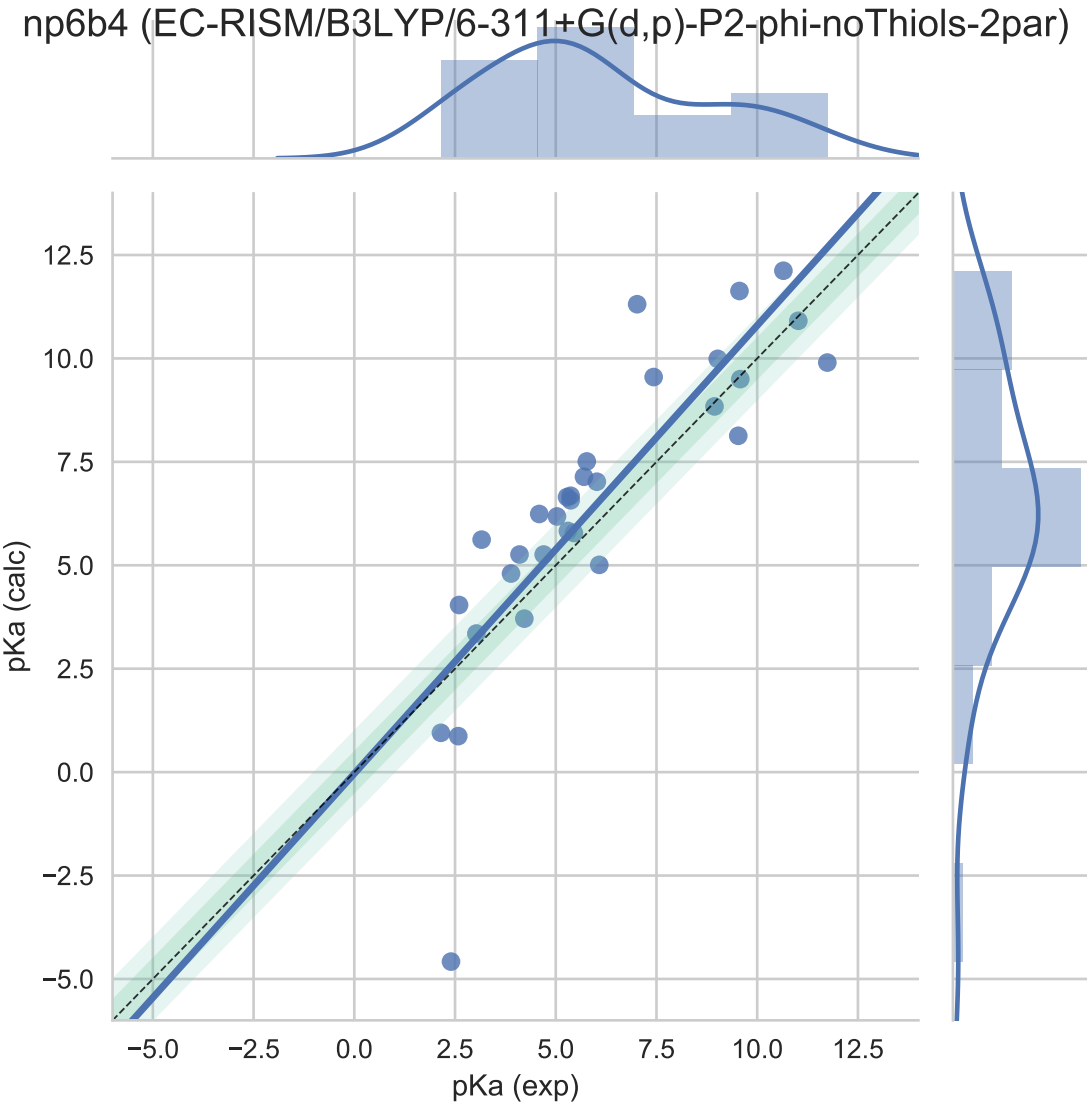
np6b4 (EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par)
pKa (calc)
pKa (exp)
12.5
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
12.5