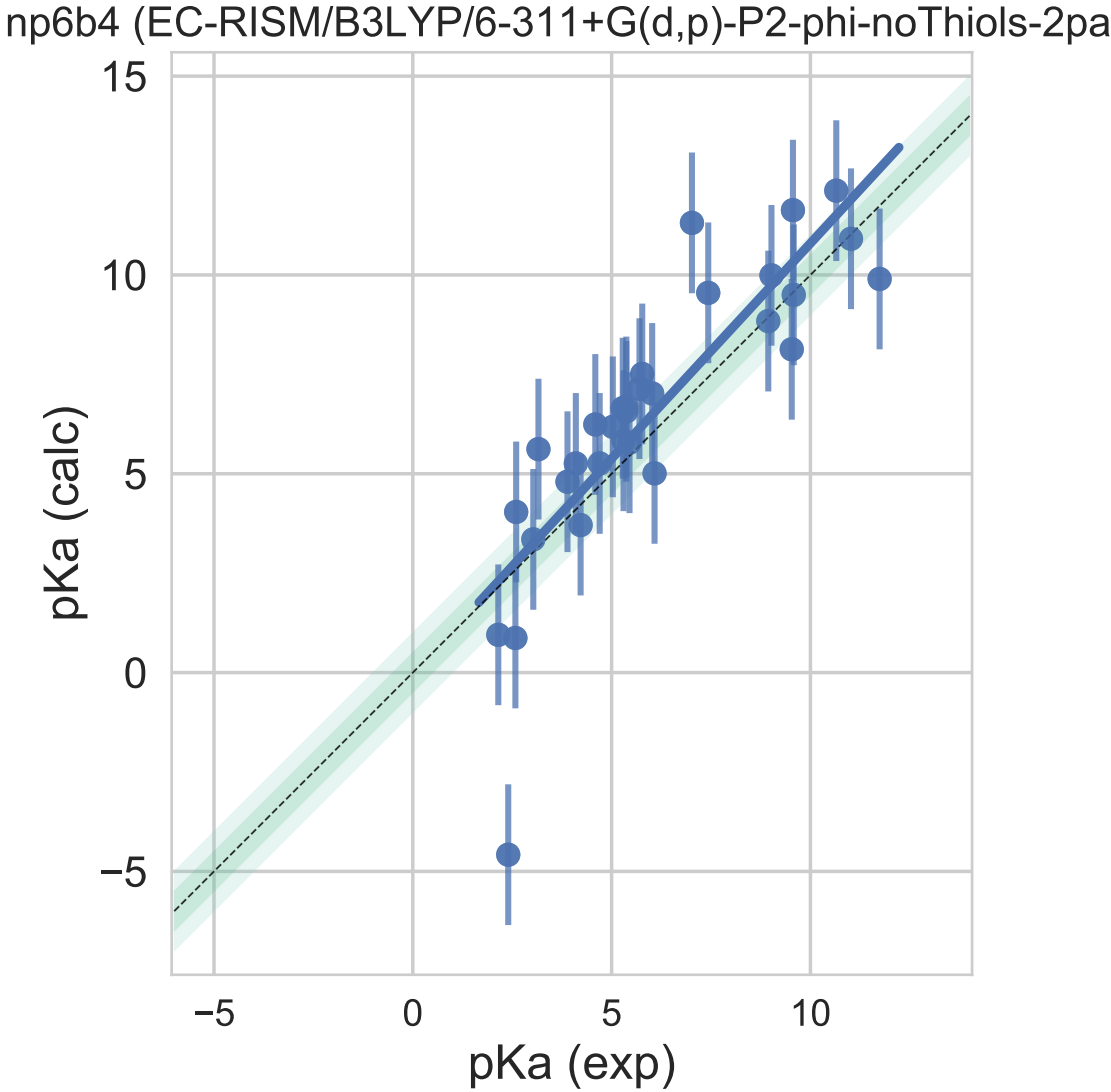
np6b4 (EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par
15
10
5
0
−5
pKa (calc)
−5
0
5
10
pKa (exp)