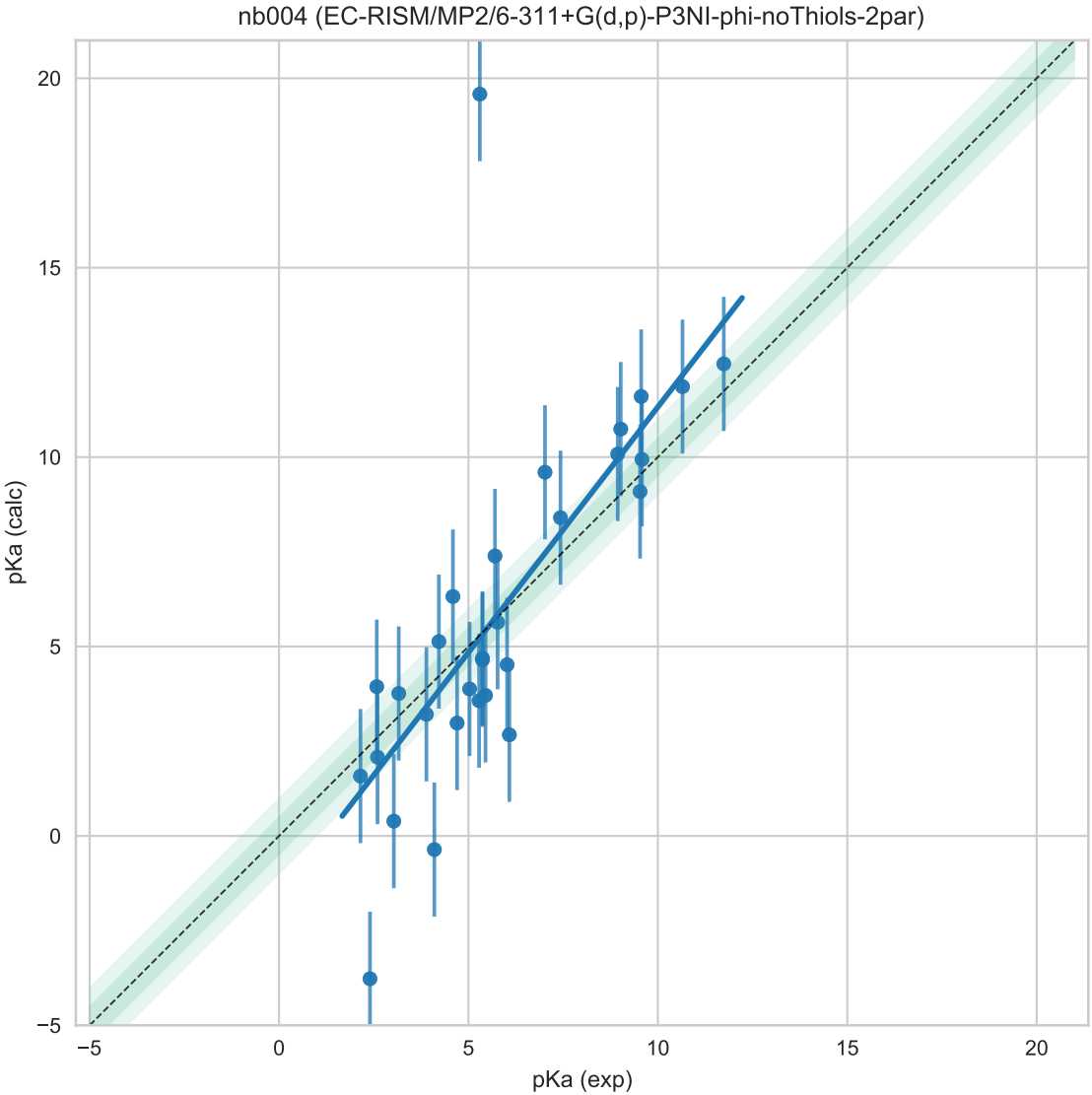
nb004 (EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par)
pKa (calc)
pKa (exp)
20
15
10
5
0
−5
−5
0
5
10
15
20