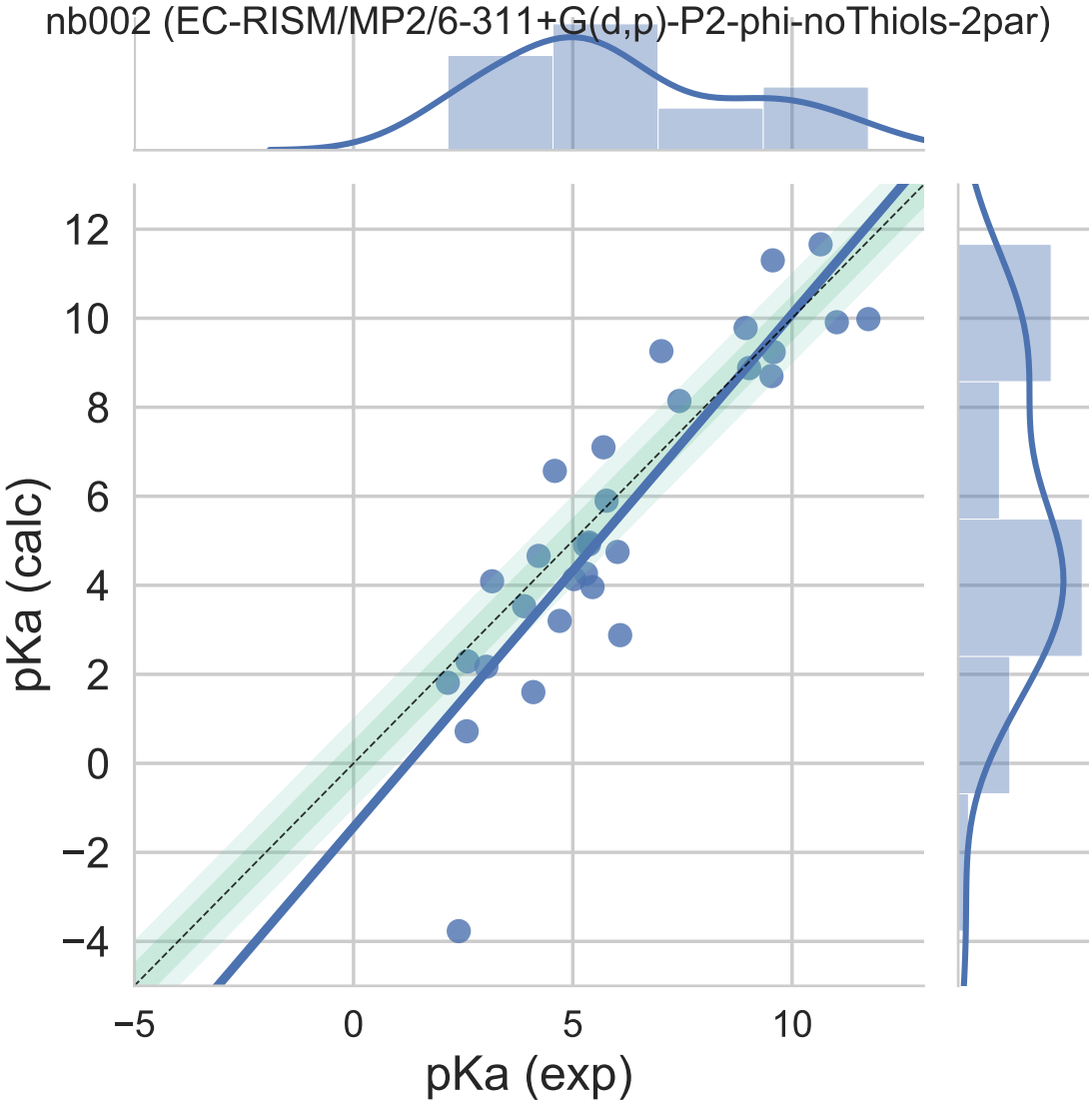
nb002 (EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par)
pKa (calc)
pKa (exp)
12
10
8
6
4
2
0
−2
−4
−5
0
5
10