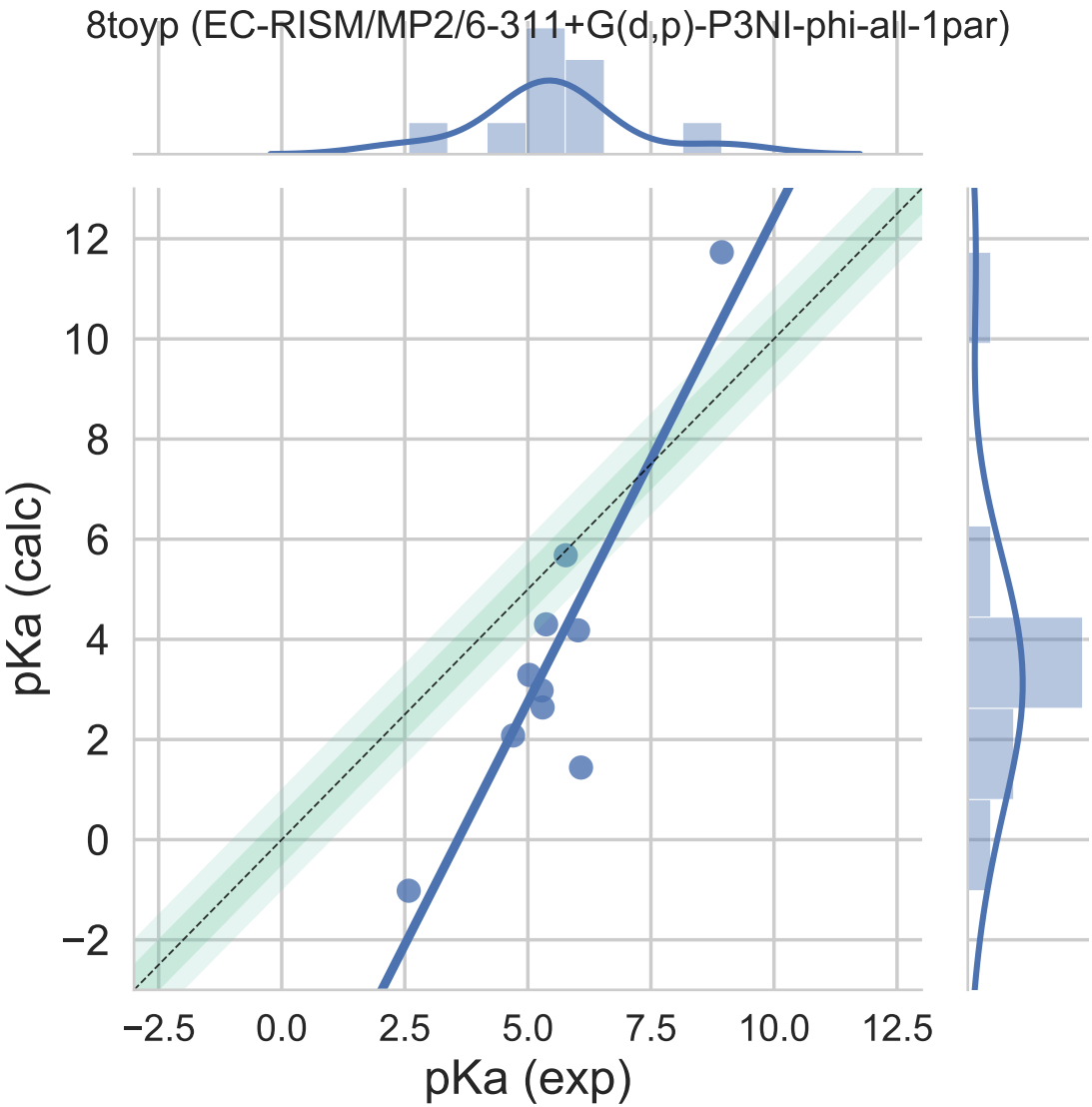
8toyp (EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par)
pKa (calc)
pKa (exp)
12
10
8
6
4
2
0
−2
−2.5
0.0
2.5
5.0
7.5
10.0
12.5