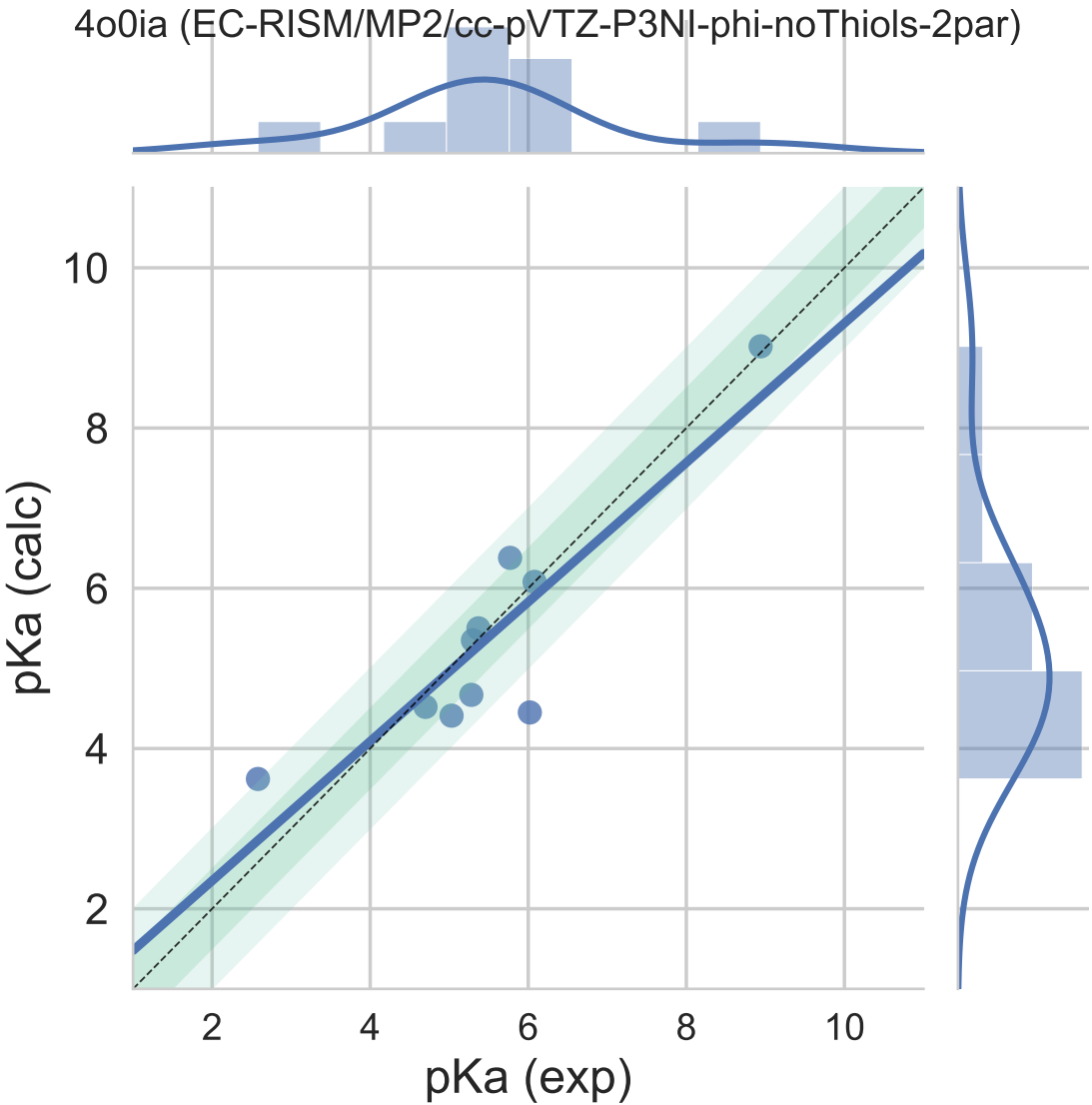
4o0ia (EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par)
pKa (calc)
pKa (exp)
2
4
6
8
10