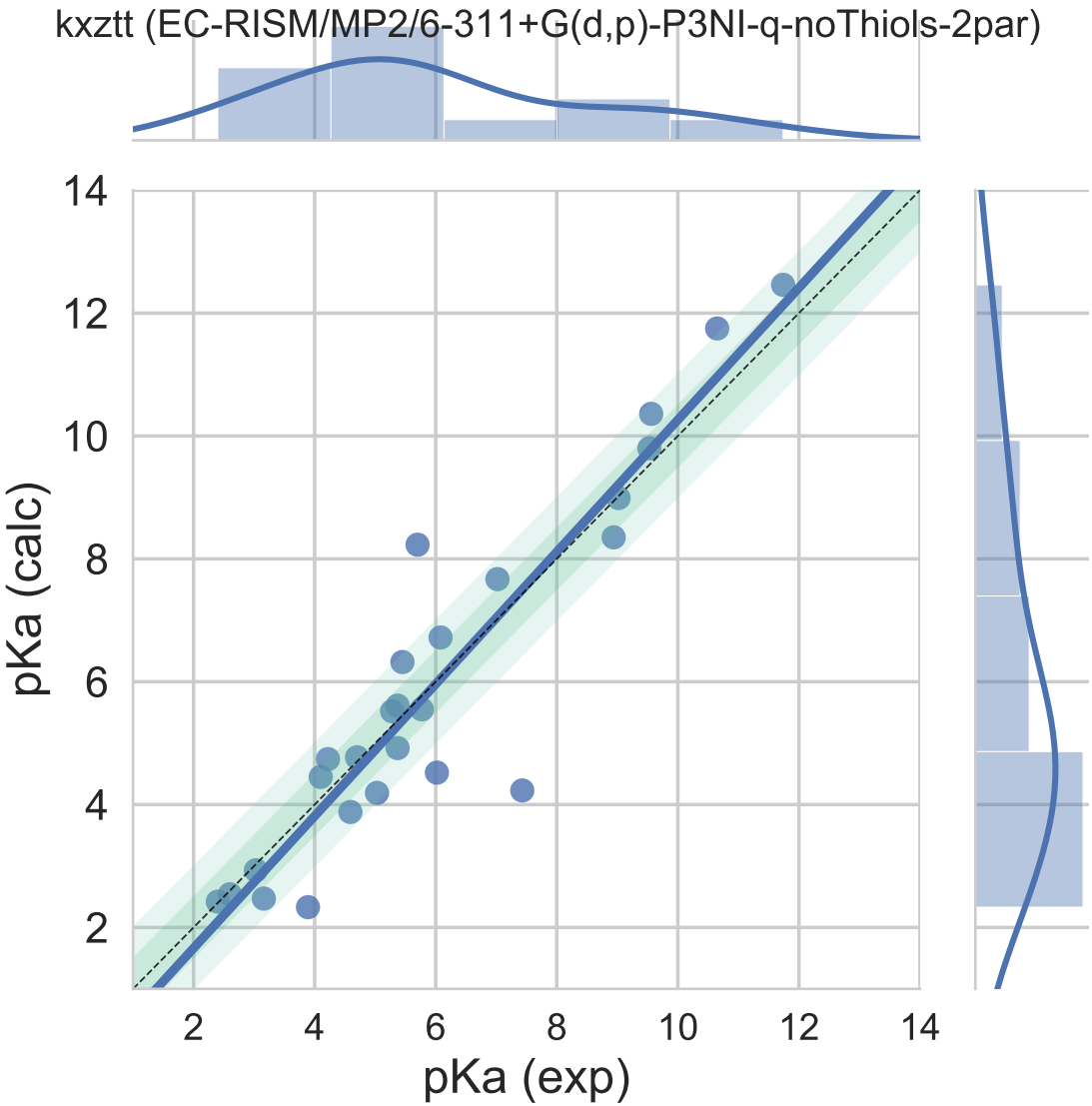
kxztt (EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par)
pKa (calc)
pKa (exp)
2
4
6
8
10
12
14