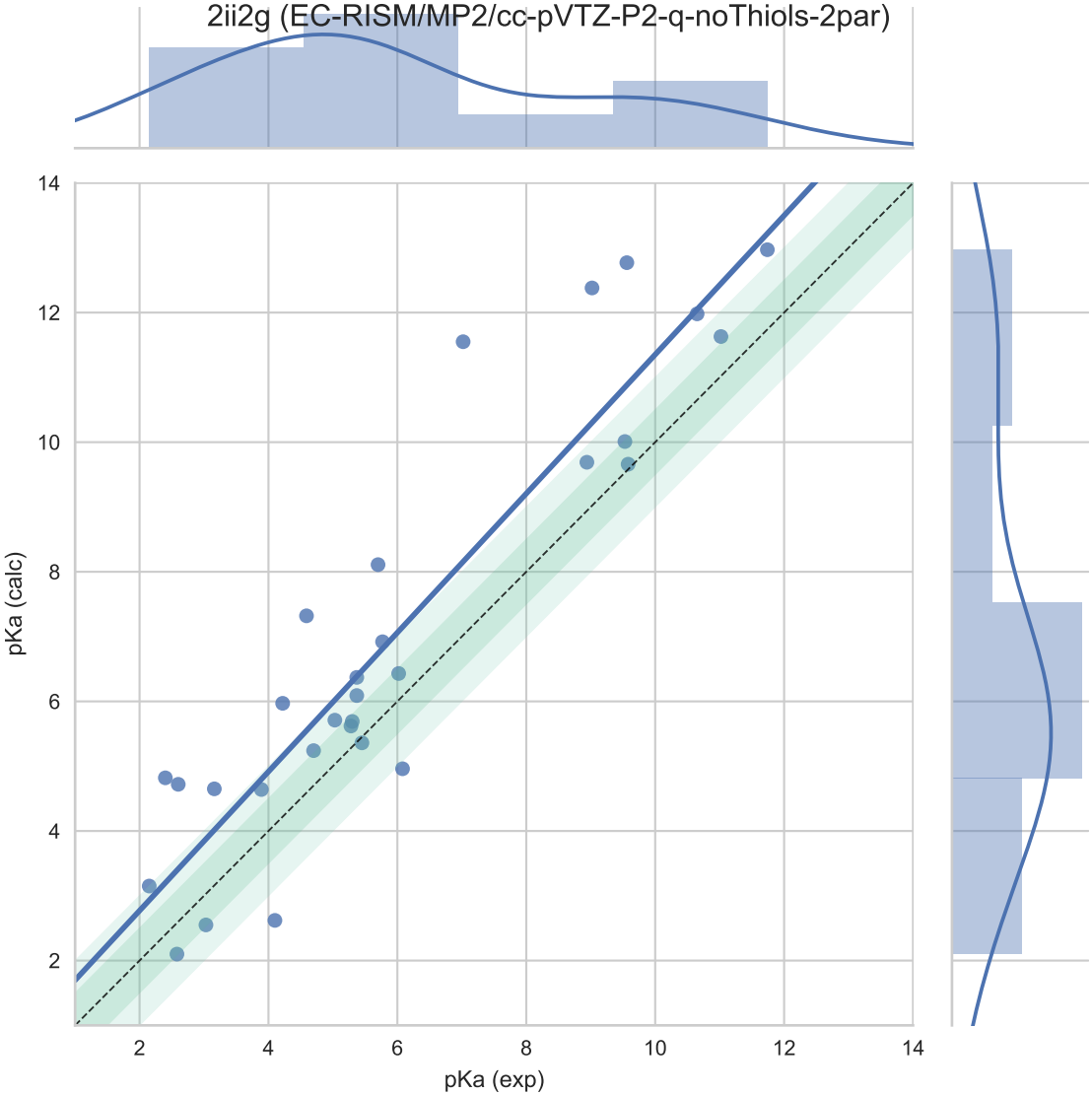
2ii2g (EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par)
pKa (calc)
pKa (exp)
2
4
6
8
10
12
14