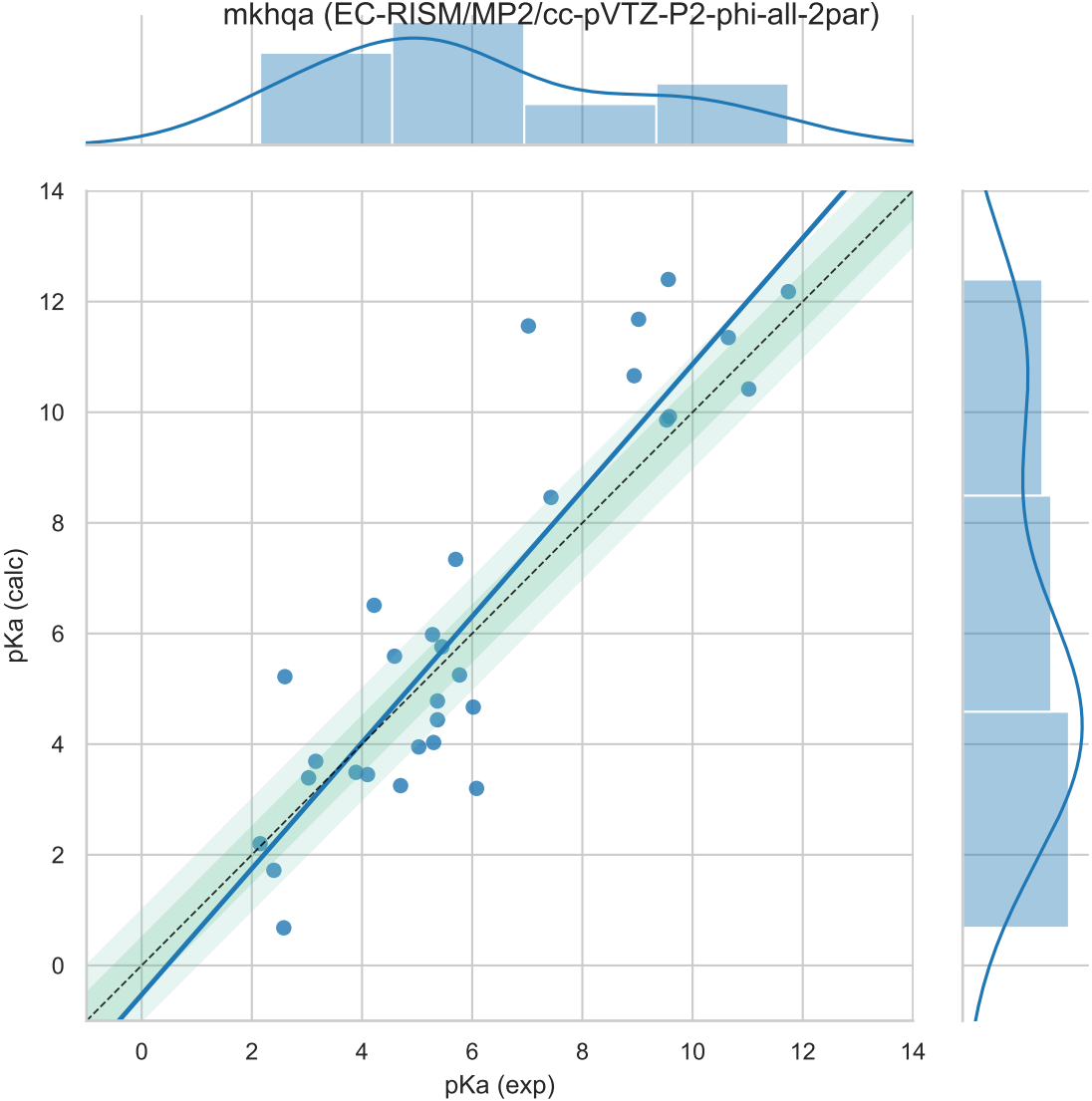
mkhqa (EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par)
pKa (calc)
pKa (exp)
0
2
4
6
8
10
12
14