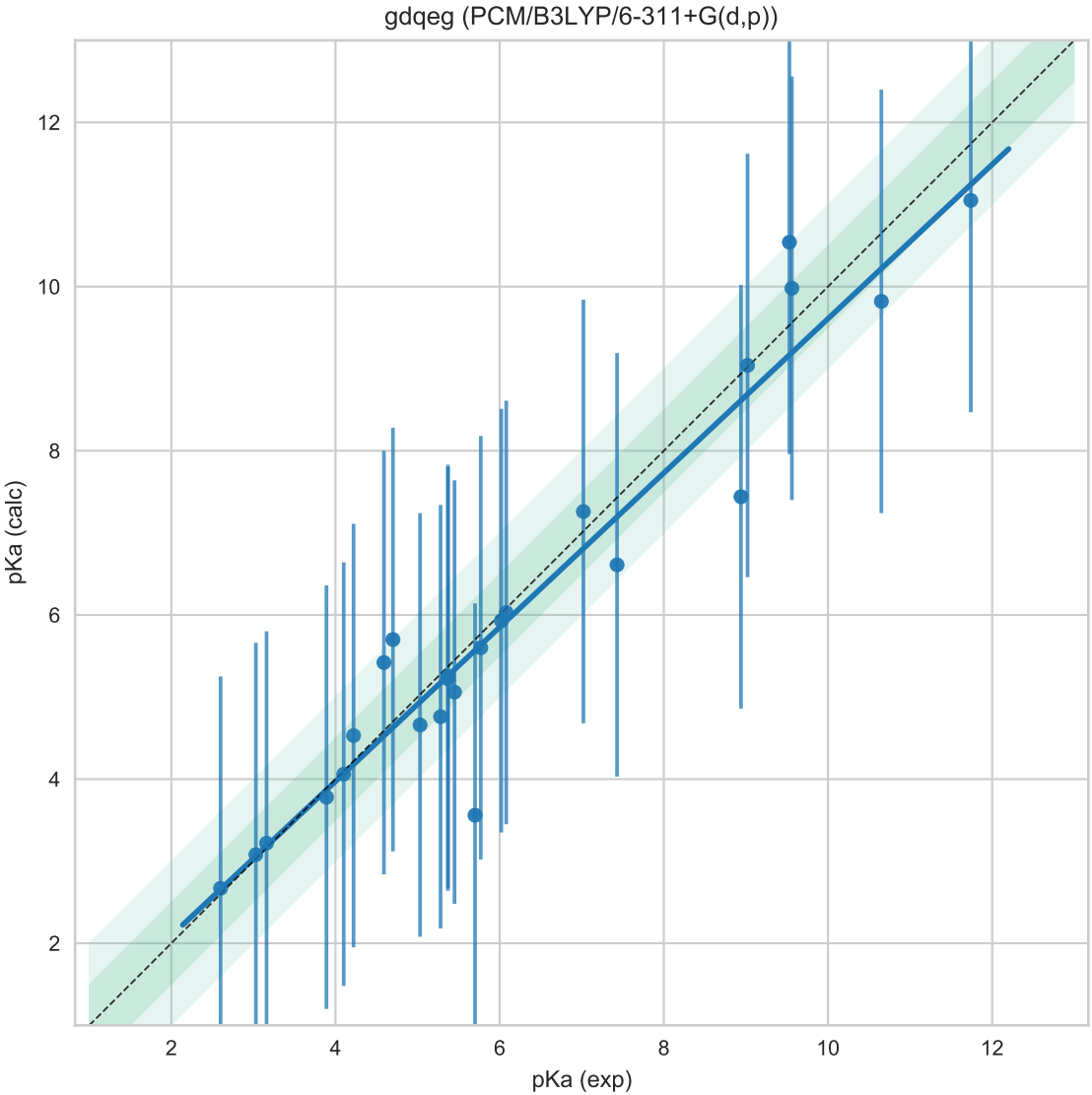
gdqeg (PCM/B3LYP/6-311+G(d,p))
pKa (calc)
pKa (exp)
2
4
6
8
10
12