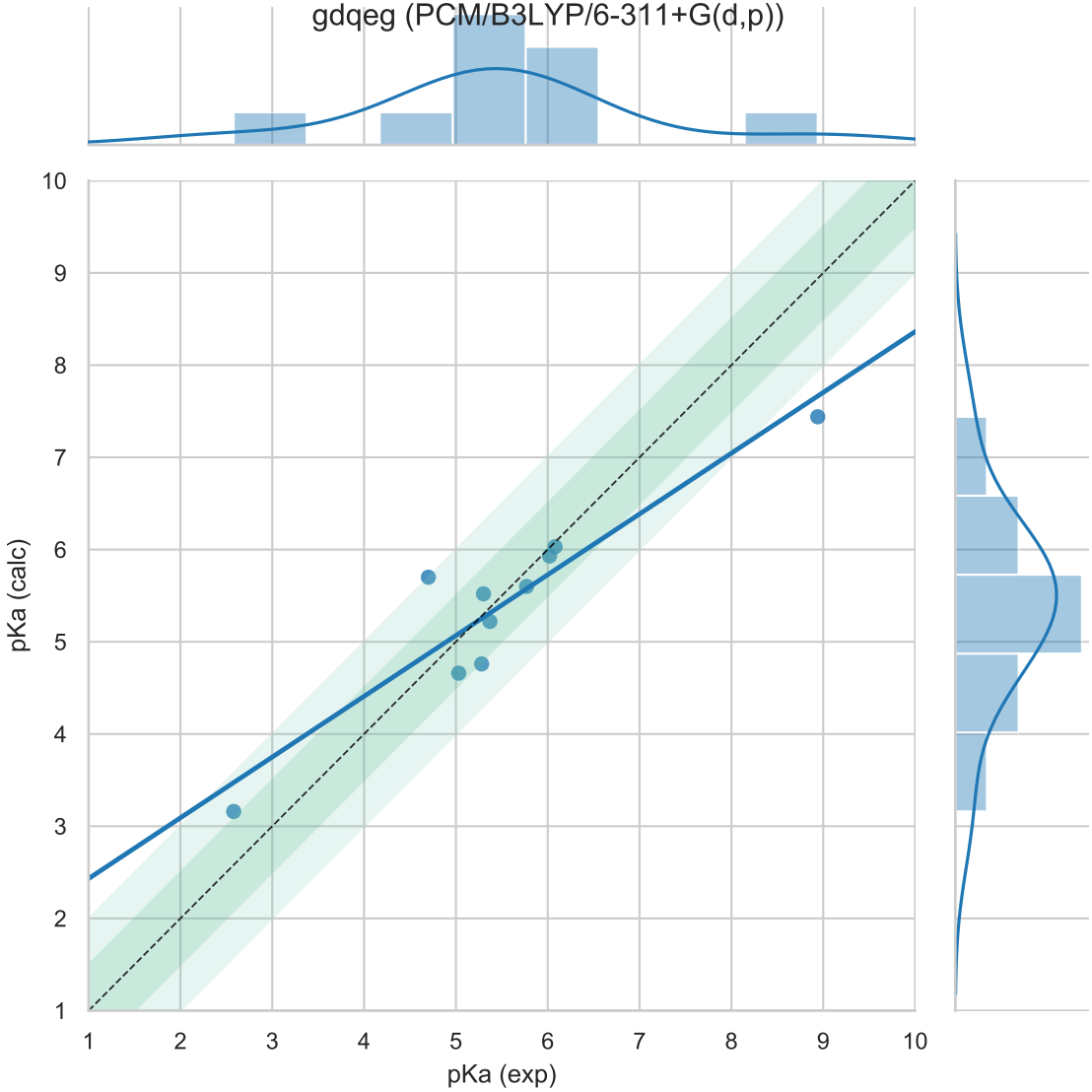
gdqeg (PCM/B3LYP/6-311+G(d,p))
pKa (calc)
pKa (exp)
1
2
3
4
5
6
7
8
9
10