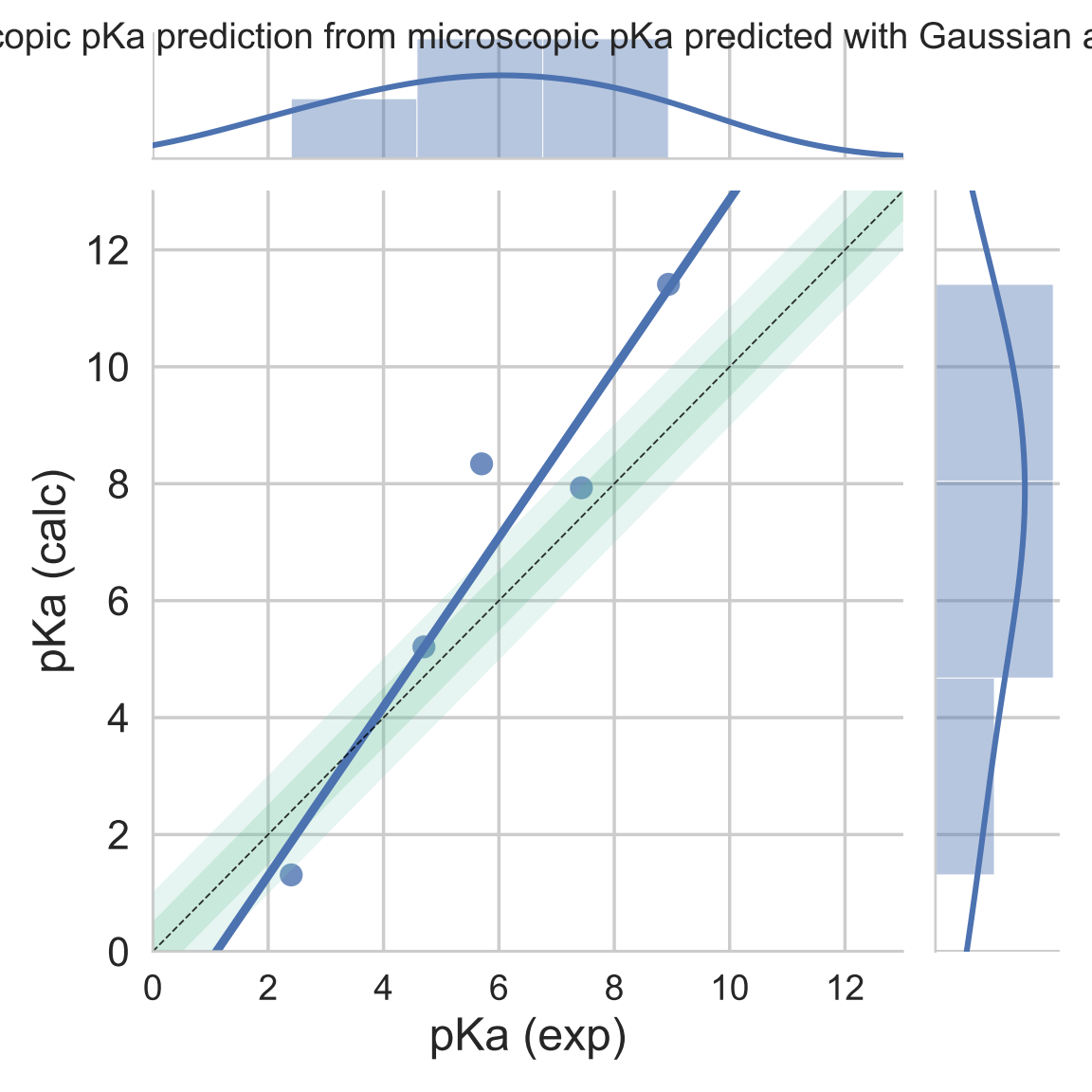
copic pKa prediction from microscopic pKa predicted with Gaussian a
pKa (calc)
pKa (exp)
0
2
4
6
8
10
12