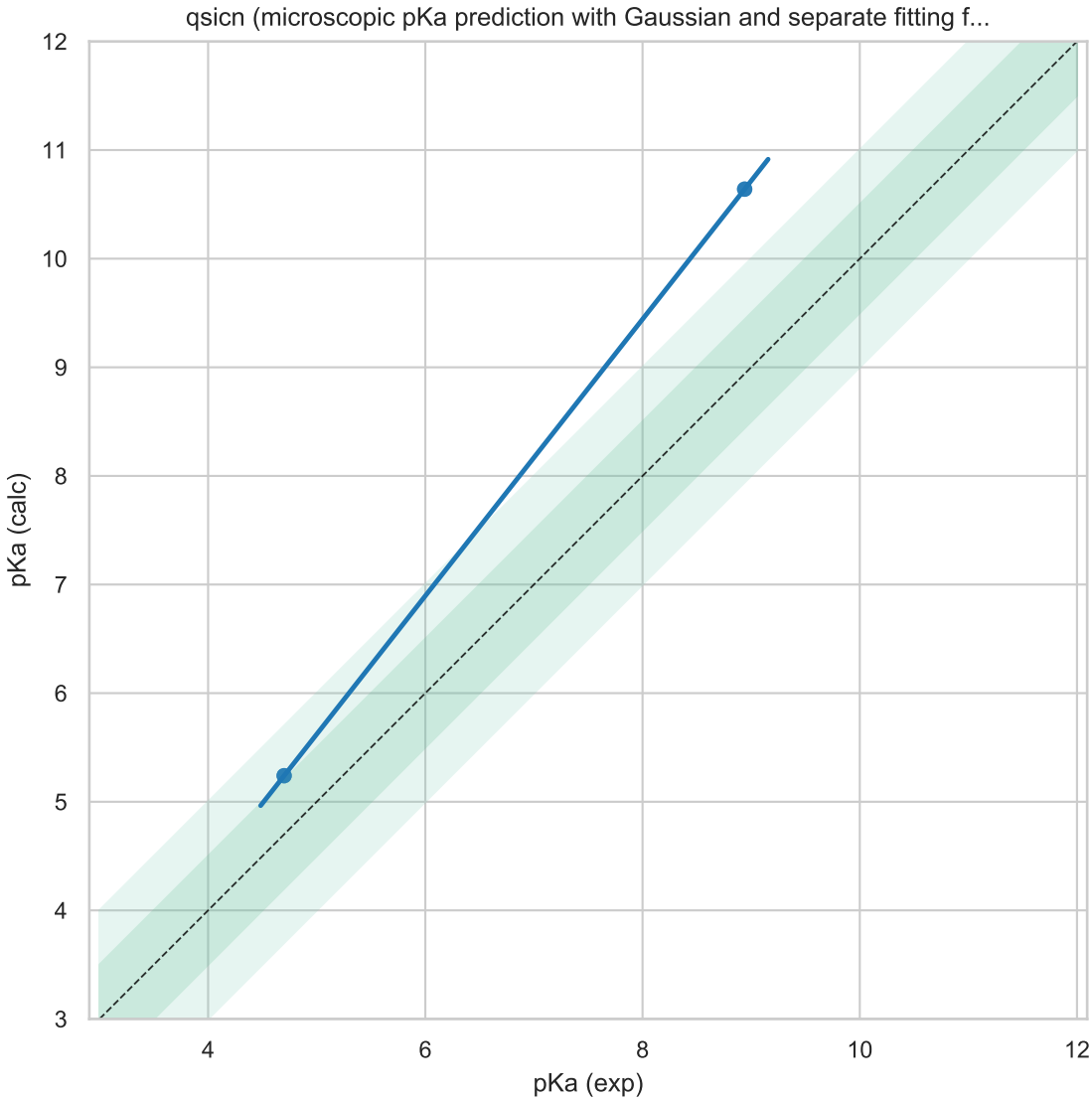
qsicn (microscopic pKa prediction with Gaussian and separate fitting f...
pKa (calc)
pKa (exp)
12
11
10
9
8
7
6
5
4
3
4
6
8
10
12