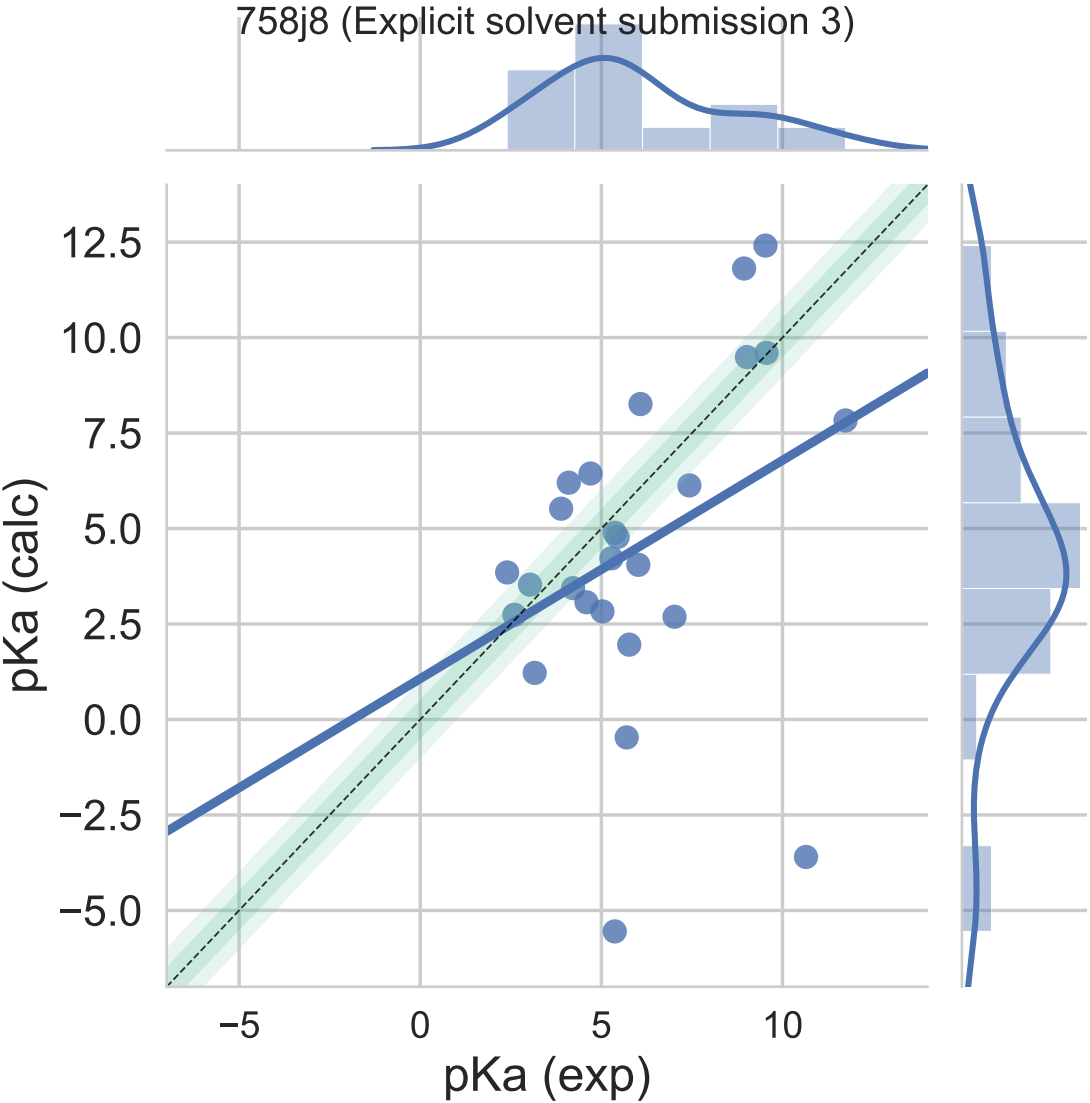
758j8 (Explicit solvent submission 3)
pKa (calc)
pKa (exp)
12.5
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−5
0
5
10