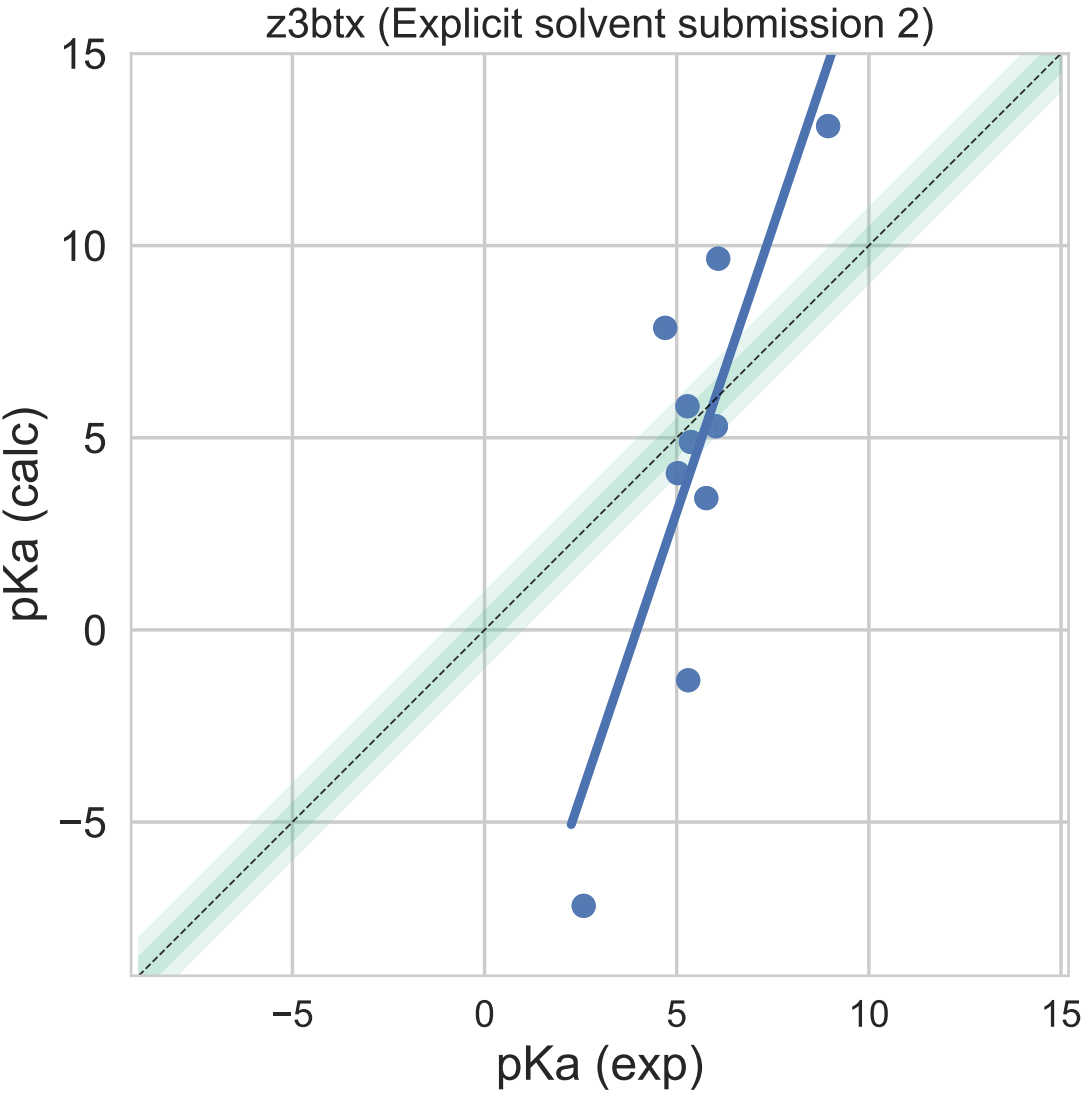
z3btx (Explicit solvent submission 2)
15
10
5
0
−5
pKa (calc)
−5
0
5
10
15
pKa (exp)