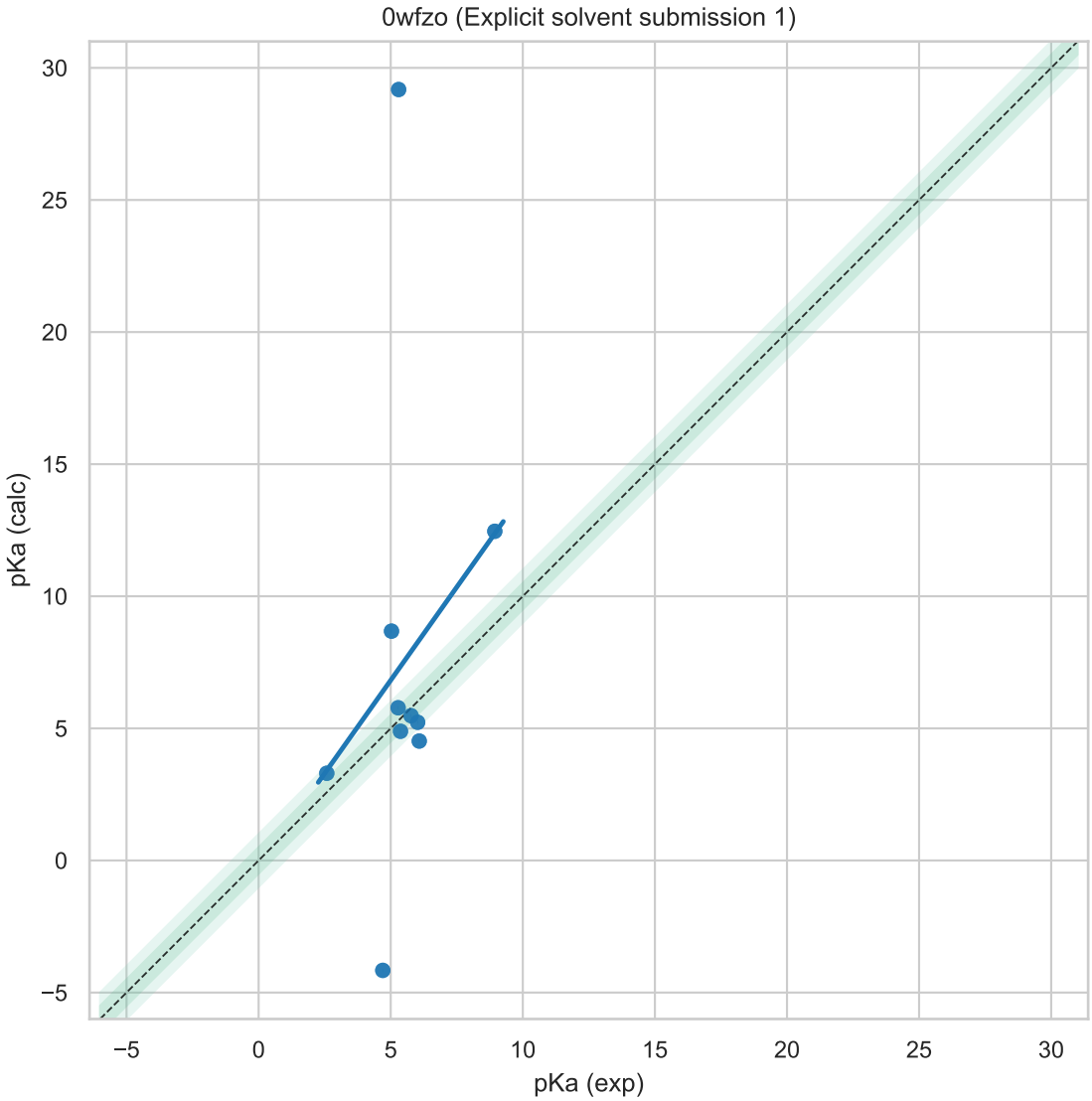
0wfzo (Explicit solvent submission 1)
pKa (calc)
pKa (exp)
30
25
20
15
10
5
0
−5
−5
0
5
10
15
20
25
30