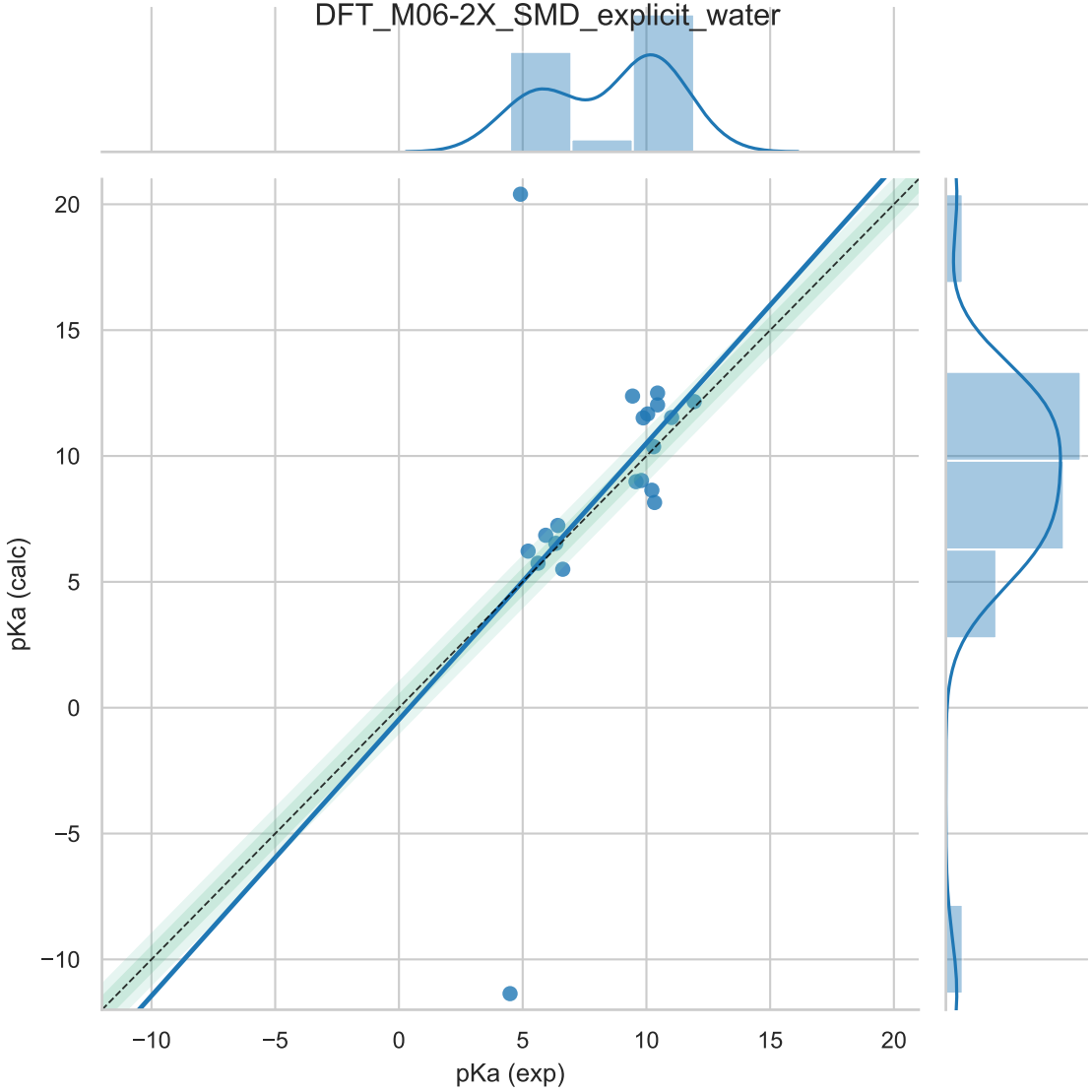
DFT_M06-2X_SMD_explicit_water
pKa (calc)
pKa (exp)
20
15
10
5
0
−5
−10
−10
−5
0
5
10
15
20