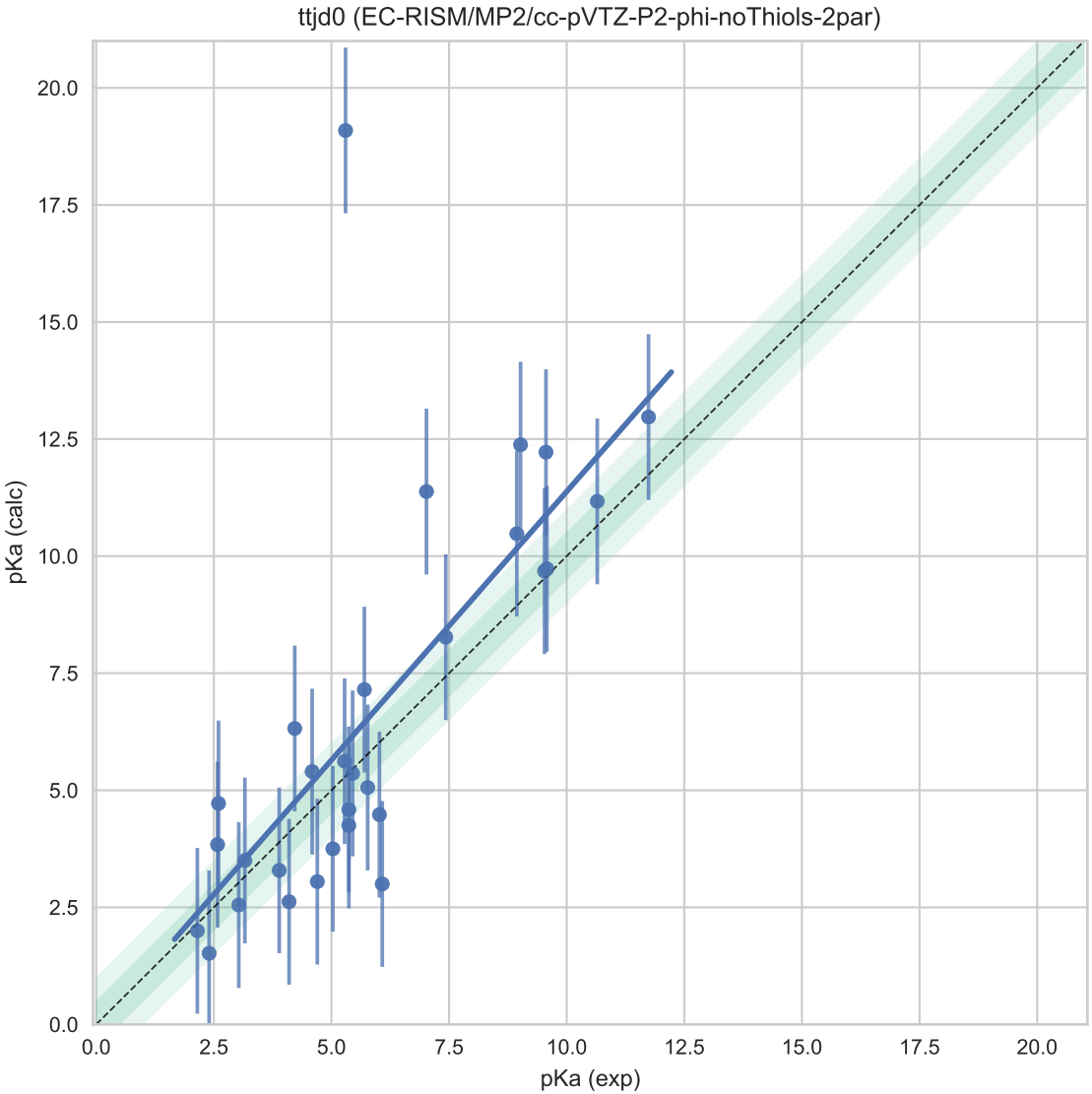
ttjd0 (EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par)
pKa (calc)
pKa (exp)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0