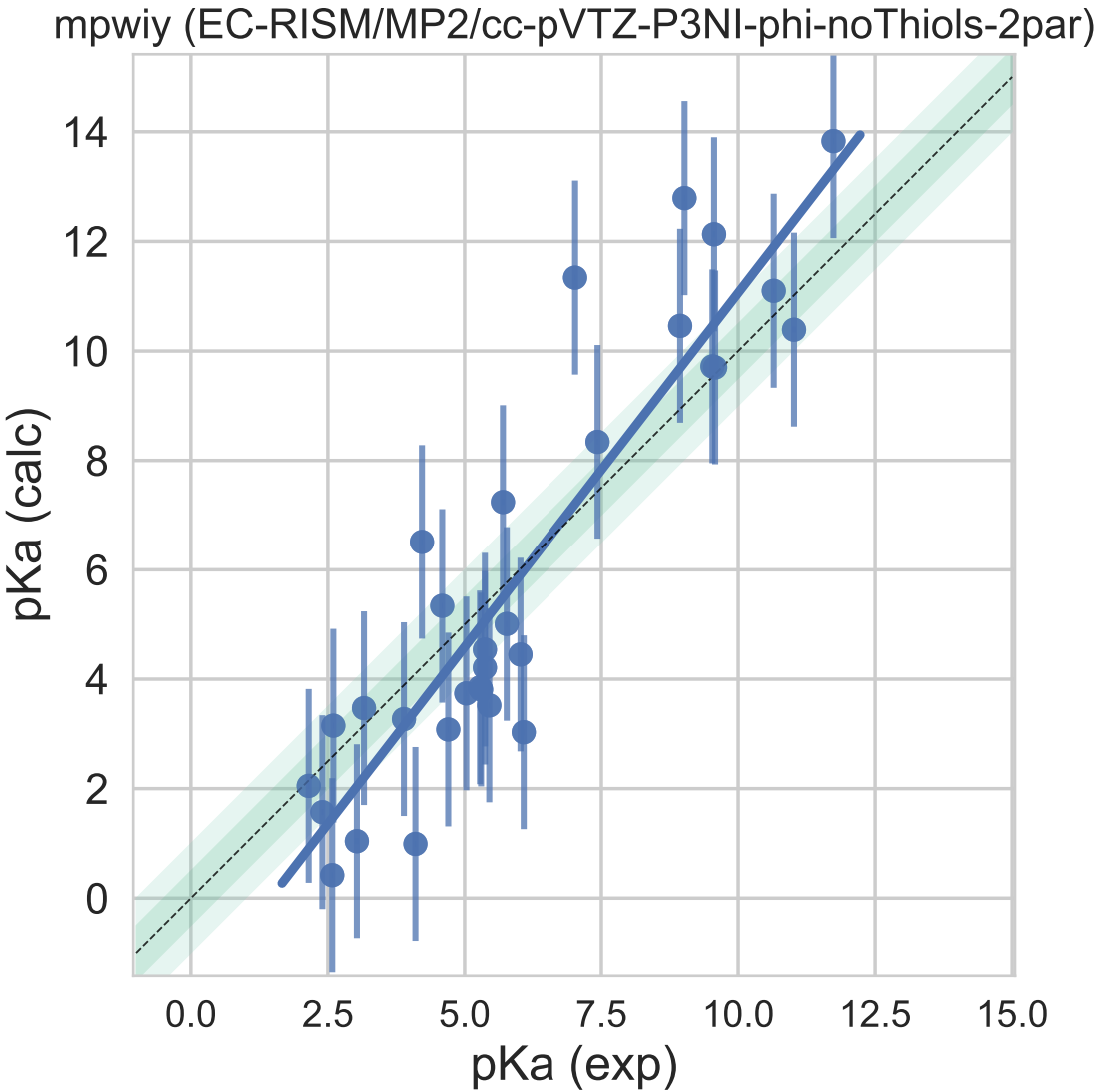
mpwiy (EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par)
pKa (calc)
pKa (exp)
0
2
4
6
8
10
12
14
0.0
2.5
5.0
7.5
10.0
12.5
15.0