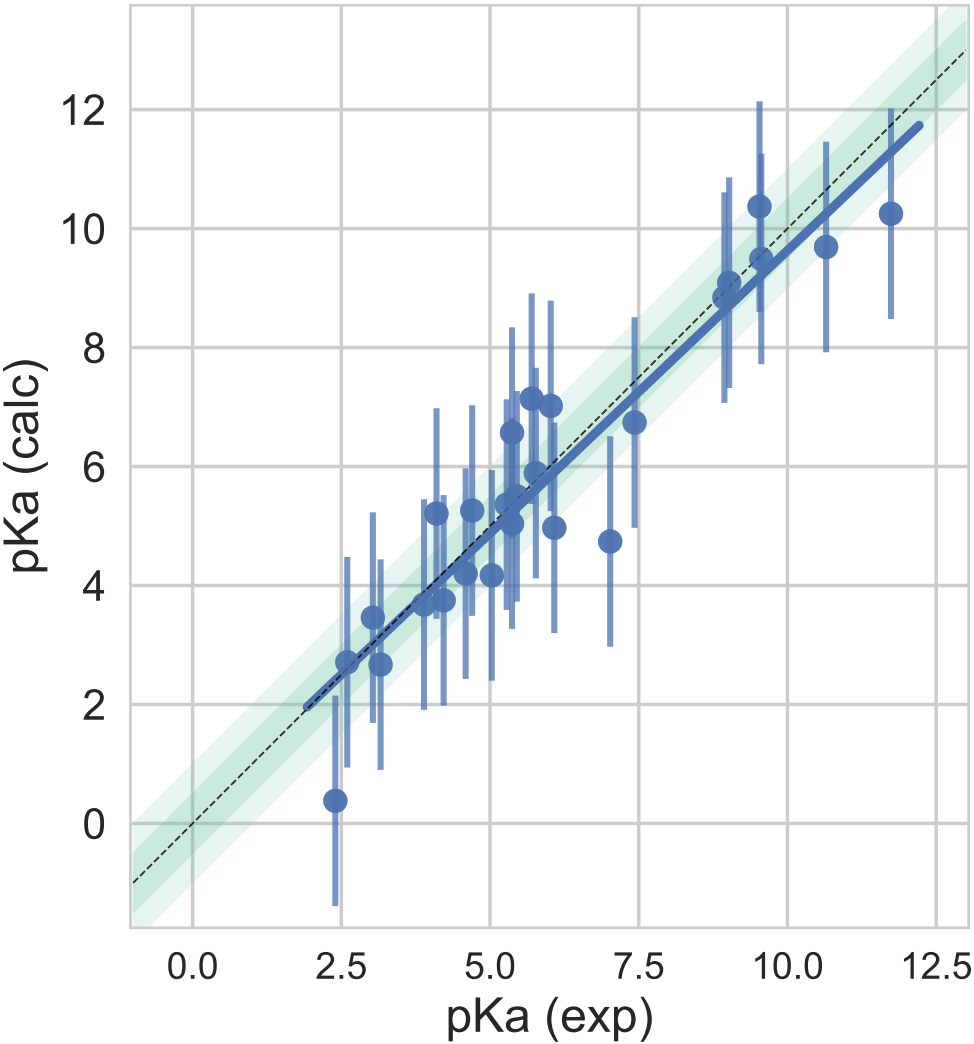cywyk (EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par)