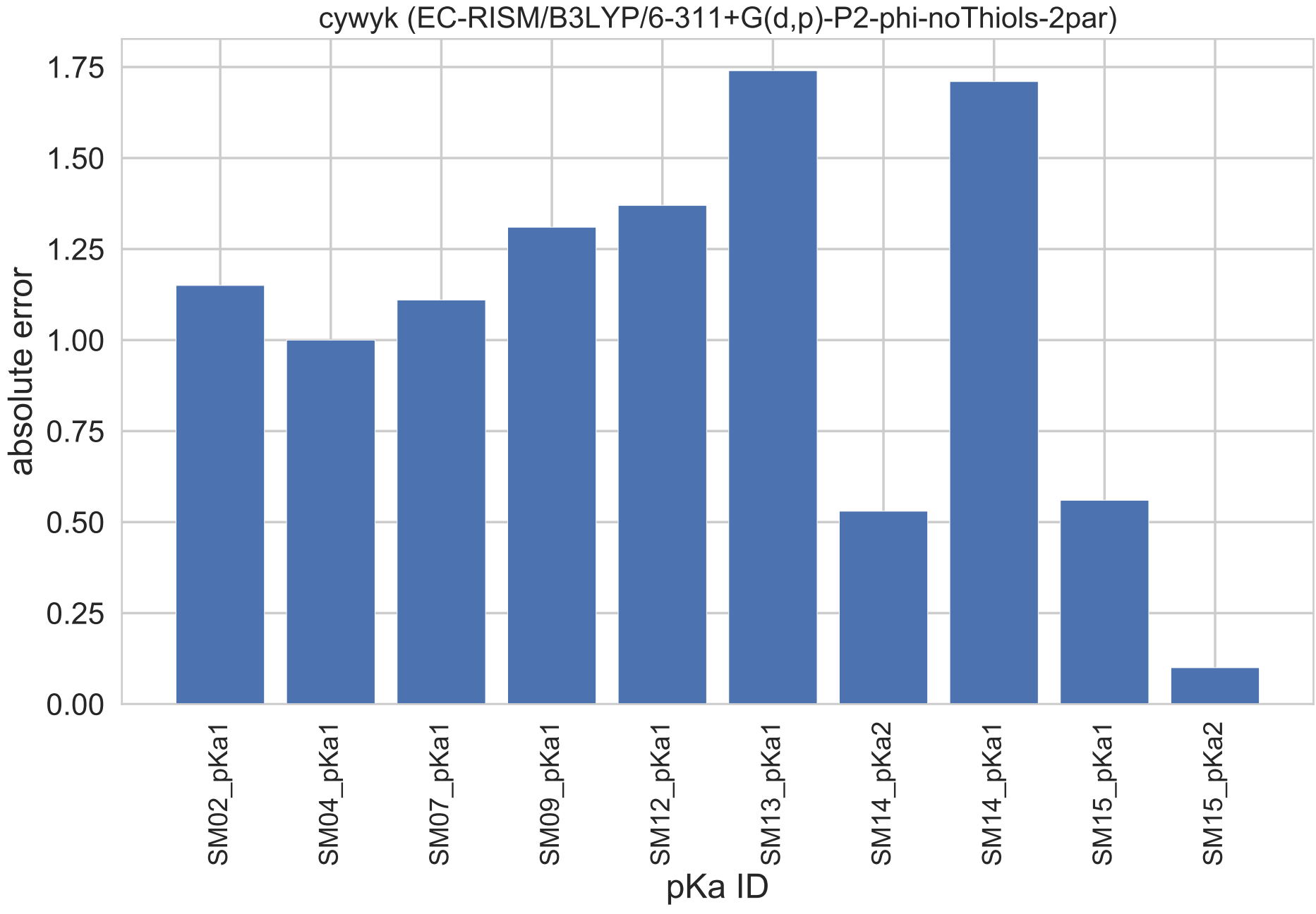
cywyk (EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par)
absolute error
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa1
SM15_pKa2
pKa ID