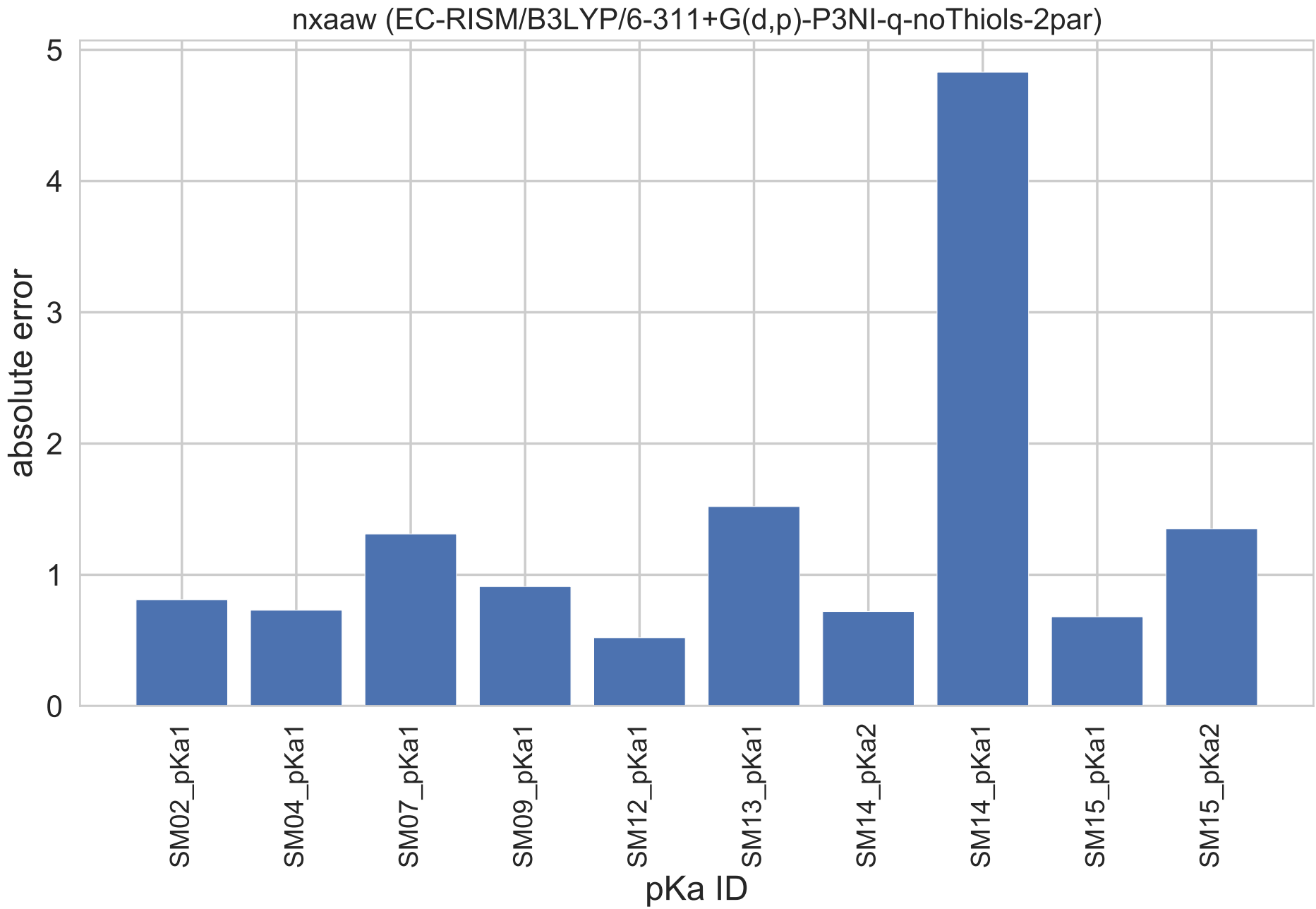
nxaaw (EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par)
absolute error
0
1
2
3
4
5
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa1
SM15_pKa2
pKa ID