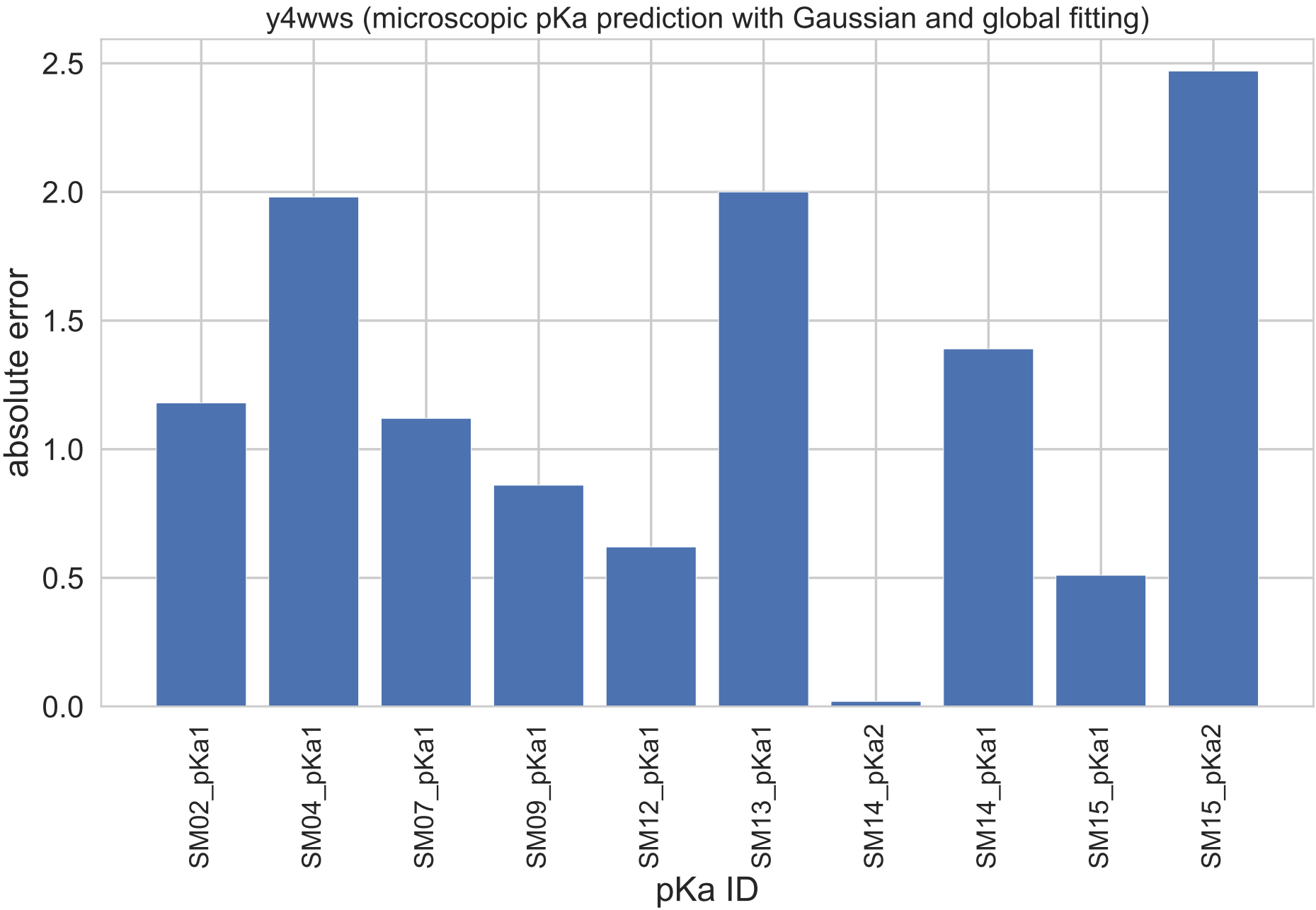
y4wws (microscopic pKa prediction with Gaussian and global fitting)
absolute error
2.5
2.0
1.5
1.0
0.5
0.0
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa1
SM15_pKa2
pKa ID