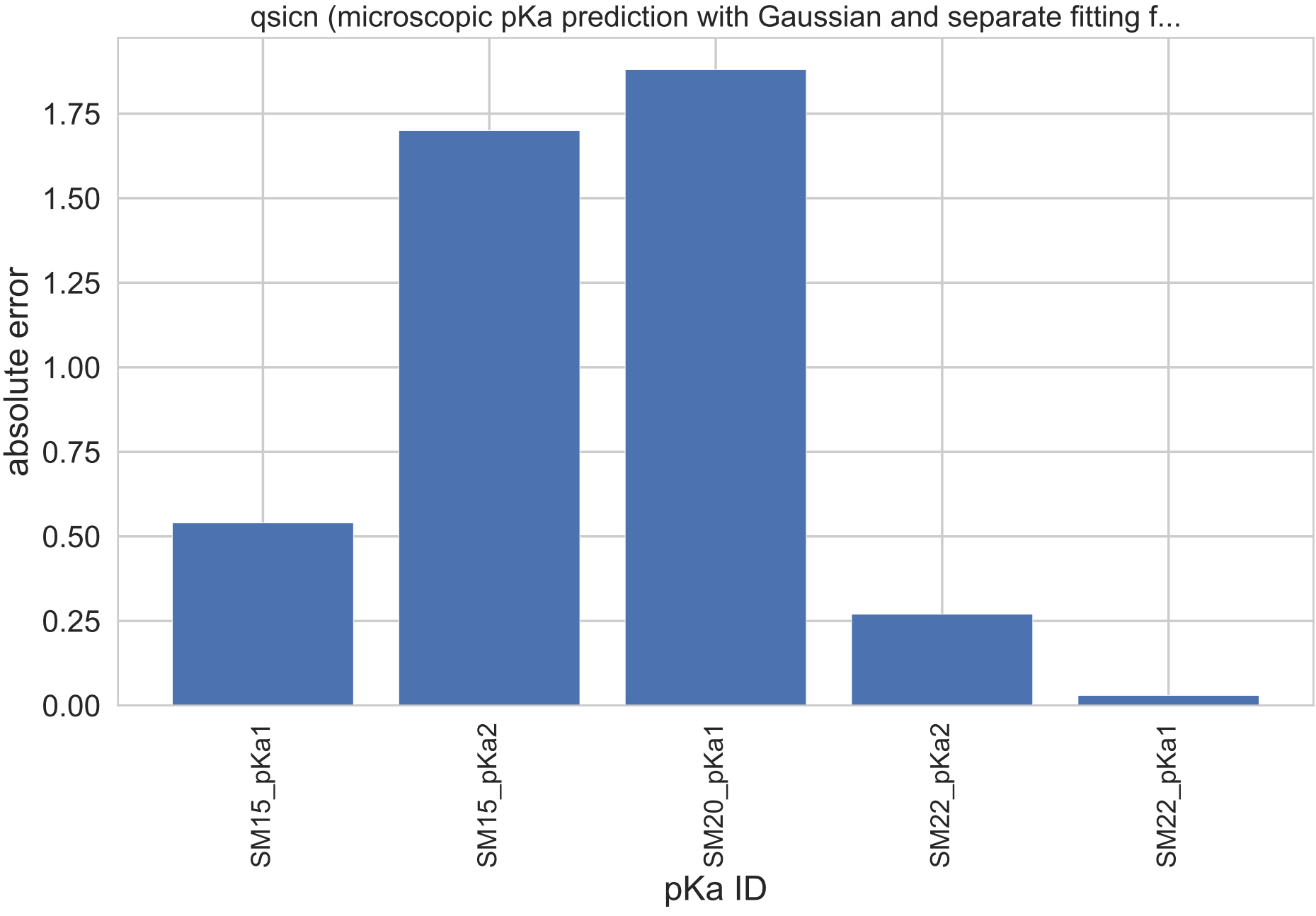
qsicn (microscopic pKa prediction with Gaussian and separate fitting f...
absolute error
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
SM15_pKa1
SM15_pKa2
SM20_pKa1
SM22_pKa2
SM22_pKa1
pKa ID