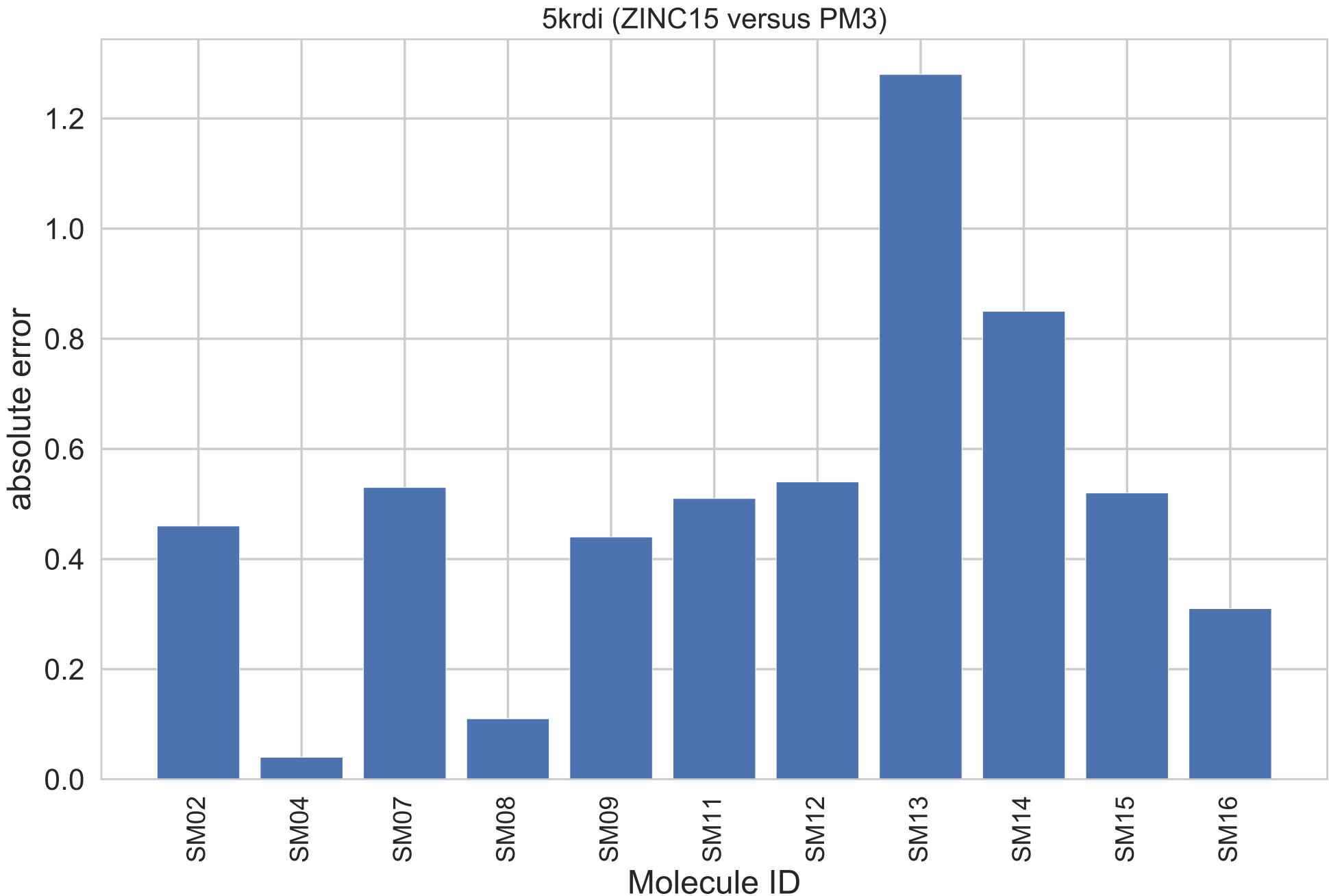
5krdi (ZINC15 versus PM3)
absolute error
0.0
0.2
0.4
0.6
0.8
1.0
1.2
SM02
SM04
SM07
SM08
SM09
SM11
SM12
SM13
SM14
SM15
SM16
Molecule ID