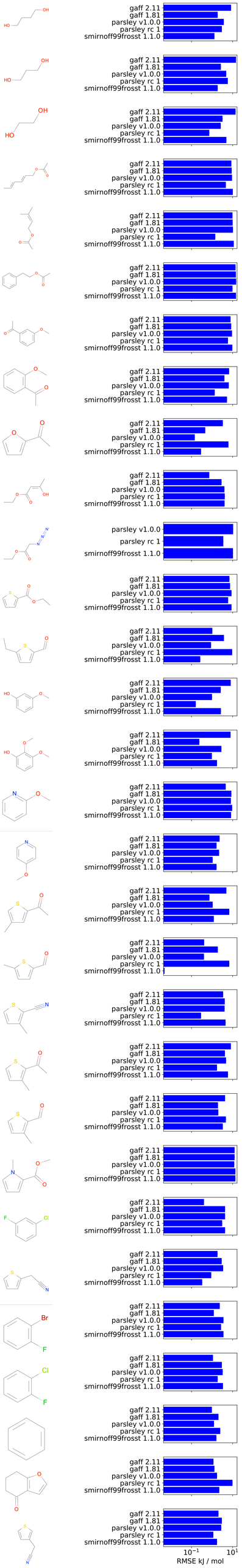
gaff 2.11
gaff 1.81
parsley v1.0.0
parsley rc 1
smirnoff99frosst 1.1.0
10^{-1}
10^{1}
RMSE kJ / mol