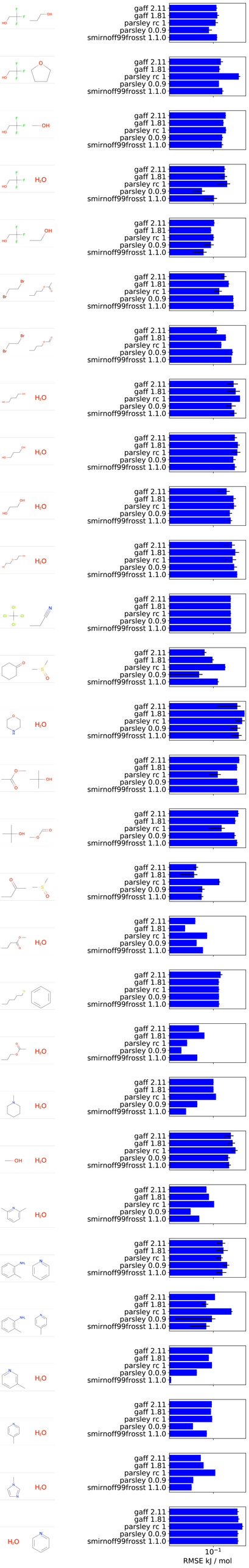
gaff 2.11
gaff 1.81
parsley rc 1
parsley 0.0.9
smirnoff99frosst 1.1.0
H2O
10−1
RMSE kJ / mol