

ID	name	RMSE	MAE	ME	R ²	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.543, 0.810]	0.579 [0.448, 0.711]	0.235 [0.001, 0.462]	0.937 [0.876, 0.973]	0.923 [0.838, 1.016]
gyuhx	S+pKa	0.730 [0.546, 0.912]	0.579 [0.426, 0.745]	0.009 [-0.258, 0.265]	0.925 [0.870, 0.964]	0.996 [0.910, 1.109]
xmyhm	ACD/pKa Classic	0.774 [0.496, 1.030]	0.546 [0.365, 0.760]	0.102 [-0.175, 0.374]	0.916 [0.832, 0.969]	0.981 [0.870, 1.107]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.681, 1.118]	0.710 [0.515, 0.922]	-0.288 [-0.582, 0.025]	0.901 [0.822, 0.953]	1.000 [0.861, 1.123]
nb017	MoKa	0.943 [0.724, 1.151]	0.770 [0.589, 0.964]	-0.162 [-0.504, 0.154]	0.884 [0.808, 0.937]	0.939 [0.823, 1.074]
nb007	Epik Scan	0.946 [0.734, 1.155]	0.776 [0.595, 0.973]	0.045 [-0.295, 0.362]	0.879 [0.761, 0.945]	0.840 [0.767, 0.920]
nb010	Epik Microscopic	1.028 [0.773, 1.272]	0.814 [0.604, 1.049]	0.243 [-0.122, 0.586]	0.869 [0.768, 0.940]	0.946 [0.825, 1.074]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.779, 1.356]	0.814 [0.575, 1.070]	-0.475 [-0.820, -0.141]	0.906 [0.841, 0.951]	1.078 [0.934, 1.216]
nb013	Jaguar	1.103 [0.719, 1.468]	0.803 [0.563, 1.091]	-0.148 [-0.551, 0.213]	0.884 [0.784, 0.948]	1.092 [0.906, 1.256]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.984, 1.568]	1.044 [0.795, 1.307]	0.129 [-0.334, 0.565]	0.874 [0.800, 0.932]	1.162 [0.941, 1.339]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.708, 1.728]	1.084 [0.428, 1.720]	-0.924 [-1.720, -0.108]	0.910 [0.509, 1.000]	1.185 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.858, 1.808]	0.955 [0.637, 1.323]	-0.101 [-0.587, 0.398]	0.854 [0.727, 0.939]	1.171 [0.999, 1.349]
hytjn	OE Gaussian Process	1.434 [0.991, 1.820]	1.034 [0.689, 1.410]	0.240 [-0.287, 0.764]	0.675 [0.423, 0.853]	0.849 [0.556, 1.100]
q3pfp	OE Gaussian Process Resampled	1.484 [1.063, 1.875]	1.140 [0.806, 1.510]	0.090 [-0.429, 0.670]	0.667 [0.428, 0.838]	0.886 [0.589, 1.172]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.146, 2.038]	1.239 [0.909, 1.618]	-0.316 [-0.879, 0.226]	0.803 [0.672, 0.901]	1.140 [0.979, 1.340]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.215, 2.135]	1.304 [0.957, 1.700]	-1.061 [-1.543, -0.614]	0.837 [0.733, 0.916]	1.073 [0.932, 1.254]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.060, 2.390]	1.219 [0.843, 1.678]	0.422 [-0.127, 1.043]	0.792 [0.687, 0.901]	1.192 [0.969, 1.489]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	-1.006 [-2.178, 0.136]	0.919 [0.463, 1.000]	1.446 [0.735, 2.147]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.085, 2.409]	1.250 [0.882, 1.723]	0.467 [-0.091, 1.094]	0.794 [0.687, 0.901]	1.200 [0.976, 1.492]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.359, 2.108]	1.436 [1.086, 1.802]	1.227 [0.781, 1.676]	0.922 [0.861, 0.962]	1.299 [1.131, 1.465]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.589, 2.141]	1.674 [1.358, 1.980]	-0.688 [-1.293, -0.021]	0.531 [0.337, 0.721]	0.670 [0.427, 0.987]
5byn6	Adiabatic scheme for type III submission	1.891 [1.486, 2.273]	1.553 [1.177, 1.945]	1.273 [0.772, 1.777]	0.912 [0.841, 0.959]	1.346 [1.162, 1.522]
y75vj	Direct scheme for type III submission	1.901 [1.504, 2.268]	1.584 [1.219, 1.969]	1.039 [0.466, 1.600]	0.891 [0.792, 0.950]	1.345 [1.161, 1.528]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.211, 2.730]	1.435 [1.038, 1.949]	-0.467 [-1.069, 0.244]	0.709 [0.601, 0.869]	1.083 [0.805, 1.449]
w4iyd	Vertical scheme for type III submission	1.939 [1.533, 2.317]	1.578 [1.183, 2.001]	1.211 [0.666, 1.761]	0.849 [0.713, 0.929]	1.256 [1.015, 1.453]
pwn3m	Analog_search	1.970 [0.770, 2.861]	1.115 [0.571, 1.807]	0.285 [-0.383, 1.103]	0.354 [0.014, 0.899]	0.583 [0.070, 1.039]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.379, 2.950]	1.578 [1.096, 2.152]	-0.733 [-1.422, 0.035]	0.769 [0.671, 0.891]	1.291 [1.010, 1.644]
xikp8	Direct scheme with single point correction for...	2.340 [1.915, 2.729]	2.026 [1.612, 2.452]	0.933 [0.142, 1.682]	0.867 [0.768, 0.933]	1.524 [1.290, 1.782]
5nm4j	Substructure matches from experimental data	2.450 [1.396, 3.338]	1.583 [0.936, 2.347]	0.046 [-0.804, 1.050]	0.192 [0.002, 0.703]	0.398 [-0.066, 0.828]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.620, 3.300]	1.744 [1.158, 2.426]	-0.526 [-1.373, 0.397]	0.726 [0.592, 0.848]	1.373 [1.034, 1.787]
0hxtm	COSMOtherm_FINE17	2.638 [0.906, 3.816]	1.423 [0.677, 2.372]	0.736 [-0.114, 1.802]	0.127 [0.000, 0.821]	0.406 [-0.241, 1.043]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.443, 4.625]	1.883 [1.231, 2.856]	-0.230 [-1.440, 0.721]	0.540 [0.238, 0.881]	1.171 [0.952, 1.379]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.280, 4.710]	1.695 [1.013, 2.697]	-0.773 [-1.914, 0.115]	0.516 [0.218, 0.886]	1.147 [0.956, 1.353]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.459, 4.647]	1.841 [1.175, 2.814]	-0.491 [-1.676, 0.430]	0.547 [0.258, 0.876]	1.192 [0.988, 1.421]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.497, 5.077]	1.985 [1.230, 3.078]	-0.102 [-1.422, 0.957]	0.523 [0.232, 0.872]	1.296 [1.033, 1.599]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.487, 5.063]	1.997 [1.242, 3.051]	-0.138 [-1.400, 0.919]	0.526 [0.234, 0.873]	1.305 [1.040, 1.605]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.883, 6.435]	2.443 [1.513, 3.851]	-0.470 [-2.110, 0.802]	0.486 [0.190, 0.877]	1.435 [1.129, 1.763]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.438, 6.836]	2.999 [1.996, 4.371]	-0.370 [-2.189, 1.143]	0.517 [0.229, 0.880]	1.642 [1.329, 1.984]

Notes

- Mean and 95% confidence intervals of statistic values were calculated by bootstrapping.
- Submissions with submission IDs nb001, nb002, nb003, nb004, nb005 and nb005 include non-blind corrections to pKa predictions of only SM22 molecule. pKas of the rest of the molecules in these submissions were blindly predicted before experimental data was released.

- pKa predictions of Epik, Jaguar, Chemicalize, and MoKa were not blind (submission IDs noted as nbXXX). They were submitted after the submission deadline as reference methods.