

ID	name	RMSE	MAE	ME	R <sup>2</sup>	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.543, 0.810]	0.579 [0.450, 0.715]	0.235 [-0.003, 0.461]	0.937 [0.880, 0.972]	0.923 [0.840, 1.015]
gyuhx	S+pKa	0.730 [0.546, 0.910]	0.579 [0.425, 0.741]	0.009 [-0.261, 0.257]	0.925 [0.868, 0.963]	0.996 [0.912, 1.109]
xmyhm	ACD/pKa Classic	0.774 [0.493, 1.031]	0.546 [0.367, 0.758]	0.102 [-0.177, 0.374]	0.916 [0.830, 0.969]	0.981 [0.869, 1.108]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.684, 1.116]	0.710 [0.518, 0.914]	-0.288 [-0.581, 0.036]	0.901 [0.821, 0.953]	1.000 [0.866, 1.125]
nb017	MoKa	0.943 [0.722, 1.157]	0.770 [0.586, 0.973]	-0.162 [-0.497, 0.153]	0.884 [0.807, 0.938]	0.939 [0.823, 1.072]
nb007	Epik Scan	0.946 [0.730, 1.154]	0.776 [0.593, 0.972]	0.045 [-0.298, 0.370]	0.879 [0.764, 0.946]	0.840 [0.767, 0.923]
nb010	Epik Microscopic	1.028 [0.765, 1.264]	0.814 [0.602, 1.041]	0.243 [-0.119, 0.584]	0.869 [0.771, 0.939]	0.946 [0.824, 1.078]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.779, 1.361]	0.814 [0.580, 1.071]	-0.475 [-0.818, -0.140]	0.906 [0.840, 0.952]	1.078 [0.937, 1.219]
nb013	Jaguar	1.103 [0.711, 1.468]	0.803 [0.559, 1.089]	-0.148 [-0.557, 0.216]	0.884 [0.780, 0.947]	1.092 [0.903, 1.255]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.983, 1.563]	1.044 [0.794, 1.306]	0.129 [-0.325, 0.564]	0.874 [0.797, 0.931]	1.162 [0.937, 1.335]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.428, 1.720]	-0.924 [-1.720, -0.108]	0.910 [0.522, 1.000]	1.185 [0.339, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.846, 1.816]	0.955 [0.636, 1.339]	-0.101 [-0.601, 0.398]	0.854 [0.729, 0.940]	1.171 [0.998, 1.355]
hytjn	OE Gaussian Process	1.434 [0.986, 1.824]	1.034 [0.687, 1.416]	0.240 [-0.266, 0.775]	0.675 [0.426, 0.855]	0.849 [0.555, 1.109]
q3pfp	OE Gaussian Process Resampled	1.484 [1.053, 1.865]	1.140 [0.807, 1.506]	0.090 [-0.446, 0.640]	0.667 [0.430, 0.835]	0.886 [0.588, 1.172]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.139, 2.034]	1.239 [0.906, 1.607]	-0.316 [-0.891, 0.211]	0.803 [0.668, 0.904]	1.140 [0.983, 1.336]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.188, 2.147]	1.304 [0.940, 1.708]	-1.061 [-1.547, -0.600]	0.837 [0.729, 0.917]	1.073 [0.935, 1.254]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.057, 2.410]	1.219 [0.838, 1.693]	0.422 [-0.135, 1.049]	0.792 [0.685, 0.897]	1.192 [0.969, 1.484]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	-1.006 [-2.178, 0.134]	0.919 [0.457, 1.000]	1.446 [0.720, 2.147]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.086, 2.410]	1.250 [0.880, 1.717]	0.467 [-0.099, 1.075]	0.794 [0.686, 0.898]	1.200 [0.971, 1.491]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.357, 2.104]	1.436 [1.087, 1.796]	1.227 [0.780, 1.674]	0.922 [0.863, 0.963]	1.299 [1.129, 1.461]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.592, 2.148]	1.674 [1.365, 1.979]	-0.688 [-1.301, -0.040]	0.531 [0.337, 0.727]	0.670 [0.436, 0.982]
5byn6	Adiabatic scheme for type III submission	1.891 [1.479, 2.279]	1.553 [1.177, 1.952]	1.273 [0.772, 1.777]	0.912 [0.840, 0.958]	1.346 [1.159, 1.526]
y75vj	Direct scheme for type III submission	1.901 [1.505, 2.268]	1.584 [1.218, 1.980]	1.039 [0.452, 1.613]	0.891 [0.788, 0.951]	1.345 [1.165, 1.530]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.214, 2.734]	1.435 [1.033, 1.958]	-0.467 [-1.075, 0.237]	0.709 [0.602, 0.870]	1.083 [0.810, 1.455]
w4iyd	Vertical scheme for type III submission	1.939 [1.527, 2.307]	1.578 [1.183, 1.984]	1.211 [0.666, 1.763]	0.849 [0.713, 0.928]	1.256 [1.014, 1.453]
pwn3m	Analog_search	1.970 [0.743, 2.853]	1.115 [0.562, 1.795]	0.285 [-0.385, 1.099]	0.354 [0.014, 0.909]	0.583 [0.068, 1.038]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.368, 2.955]	1.578 [1.091, 2.154]	-0.733 [-1.424, 0.036]	0.769 [0.667, 0.890]	1.291 [1.019, 1.632]
xikp8	Direct scheme with single point correction for...	2.340 [1.895, 2.726]	2.026 [1.594, 2.456]	0.933 [0.123, 1.684]	0.867 [0.763, 0.931]	1.524 [1.290, 1.778]
5nm4j	Substructure matches from experimental data	2.450 [1.392, 3.323]	1.583 [0.933, 2.325]	0.046 [-0.822, 1.019]	0.192 [0.002, 0.707]	0.398 [-0.073, 0.823]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.618, 3.289]	1.744 [1.155, 2.428]	-0.526 [-1.381, 0.355]	0.726 [0.590, 0.849]	1.373 [1.037, 1.767]
0hxtm	COSMOtherm_FINE17	2.638 [0.882, 3.796]	1.423 [0.659, 2.354]	0.736 [-0.132, 1.793]	0.127 [0.000, 0.836]	0.406 [-0.215, 1.051]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.456, 4.614]	1.883 [1.242, 2.835]	-0.230 [-1.362, 0.717]	0.540 [0.243, 0.881]	1.171 [0.961, 1.378]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.277, 4.709]	1.695 [1.011, 2.707]	-0.773 [-1.912, 0.124]	0.516 [0.224, 0.889]	1.147 [0.953, 1.354]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.459, 4.659]	1.841 [1.173, 2.827]	-0.491 [-1.683, 0.408]	0.547 [0.249, 0.874]	1.192 [0.979, 1.421]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.501, 5.035]	1.985 [1.244, 3.040]	-0.102 [-1.354, 0.960]	0.523 [0.235, 0.871]	1.296 [1.038, 1.594]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.486, 5.092]	1.997 [1.241, 3.077]	-0.138 [-1.460, 0.918]	0.526 [0.230, 0.875]	1.305 [1.044, 1.598]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.880, 6.421]	2.443 [1.506, 3.825]	-0.470 [-2.121, 0.798]	0.486 [0.190, 0.879]	1.435 [1.126, 1.769]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.445, 6.862]	2.999 [2.001, 4.394]	-0.370 [-2.172, 1.081]	0.517 [0.221, 0.878]	1.642 [1.321, 1.982]

#### 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.