ID τ	name	RMSE	MAE	ME	R^2	m
xvxzd 0.816 [0.681, 0.917]	Full quantum chemical calculation of free ener...	0.680 [0.549, 0.812]	0.579 [0.454, 0.713]	0.235 [-0.003, 0.458]	0.937 [0.878, 0.972]	0.923 [0.837, 1.
gyuhx 0.879 [0.801, 0.943]	S+pKa	0.730 [0.548, 0.912]	0.579 [0.429, 0.744]	0.009 [-0.252, 0.268]	0.925 [0.869, 0.964]	0.996 [0.913, 1.
xmyhm 0.798 [0.667, 0.896]	ACD/pKa Classic	0.774 [0.498, 1.025]	0.546 [0.367, 0.750]	0.102 [-0.171, 0.371]	0.916 [0.833, 0.968]	0.981 [0.873, 1.
yqkga 0.838 [0.719, 0.924]	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.683, 1.127]	0.710 [0.517, 0.919]	-0.288 [-0.578, 0.035]	0.901 [0.820, 0.953]	1.000 [0.868, 1.
nb017 0.726 [0.597, 0.836]	MoKa	0.943 [0.721, 1.145]	0.770 [0.587, 0.963]	-0.162 [-0.492, 0.161]	0.884 [0.810, 0.938]	0.939 [0.822, 1.
nb007 0.787 [0.650, 0.891]	Epik Scan	0.946 [0.733, 1.156]	0.776 [0.593, 0.973]	0.045 [-0.305, 0.362]	0.879 [0.764, 0.946]	0.840 [0.767, 0.
nb010 0.800 [0.663, 0.900]	Epik Microscopic	1.028 [0.770, 1.268]	0.814 [0.603, 1.048]	0.243 [-0.106, 0.582]	0.869 [0.768, 0.939]	0.946 [0.826, 1.
8xt50 0.801 [0.687, 0.893]	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.775, 1.352]	0.814 [0.576, 1.067]	-0.475 [-0.815, -0.146]	0.906 [0.841, 0.951]	1.078 [0.937, 1.
nb013 0.792 [0.646, 0.901]	Jaguar	1.103 [0.711, 1.480]	0.803 [0.559, 1.095]	-0.148 [-0.552, 0.218]	0.884 [0.783, 0.947]	1.092 [0.905, 1.
nb015 0.775 [0.661, 0.863]	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.989, 1.579]	1.044 [0.799, 1.318]	0.129 [-0.352, 0.568]	0.874 [0.796, 0.932]	1.162 [0.941, 1.
p0jba 0.800 [0.000, 1.000]	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 [0.355, 1.
37xm8 0.732 [0.604, 0.845]	ACD/pKa GALAS	1.358 [0.844, 1.815]	0.955 [0.636, 1.330]	-0.101 [-0.598, 0.402]	0.854 [0.730, 0.939]	1.171 [0.996, 1.
hytjn 0.605 [0.336, 0.809]	OE Gaussian Process	1.434 [0.974, 1.823]	1.034 [0.672, 1.420]	0.240 [-0.274, 0.784]	0.675 [0.419, 0.859]	0.849 [0.559, 1.
q3pfp 0.638 [0.370, 0.830]	OE Gaussian Process Resampled	1.484 [1.062, 1.881]	1.140 [0.805, 1.516]	0.090 [-0.428, 0.665]	0.667 [0.427, 0.836]	0.886 [0.578, 1.
mkhqa 0.637 [0.439, 0.784]	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.138, 2.051]	1.239 [0.909, 1.618]	-0.316 [-0.885, 0.218]	0.803 [0.669, 0.903]	1.140 [0.976, 1.
2ii2g 0.700 [0.552, 0.819]	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.195, 2.141]	1.304 [0.948, 1.701]	-1.061 [-1.540, -0.590]	0.837 [0.731, 0.916]	1.073 [0.933, 1.
nb001 0.713 [0.527, 0.842]	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.058, 2.397]	1.219 [0.842, 1.693]	0.422 [-0.130, 1.068]	0.792 [0.684, 0.899]	1.192 [0.971, 1.
35bdm 0.800 [0.000, 1.000]	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 [0.463, 1.000]	1.446 [0.735, 2.
nb002 0.723 [0.547, 0.851]	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.085, 2.406]	1.250 [0.879, 1.708]	0.467 [-0.089, 1.079]	0.794 [0.689, 0.900]	1.200 [0.974, 1.
ryzue 0.829 [0.710, 0.922]	Adiabatic scheme with single point correction ...	1.745 [1.364, 2.101]	1.436 [1.090, 1.794]	1.227 [0.776, 1.664]	0.922 [0.861, 0.962]	1.299 [1.131, 1.
yc70m 0.568 [0.378, 0.723]	PCM/B3LYP/6-311+G(d,p)	1.878 [1.593, 2.149]	1.674 [1.364, 1.982]	-0.688 [-1.303, -0.036]	0.531 [0.333, 0.724]	0.670 [0.428, 0.

Continued on next page

ID	name	RMSE	MAE	ME	R^2	m	τ
5byn6	Adiabatic scheme for type III submission	1.891 [1.489, 2.278]	1.553 [1.179, 1.953]	1.273 [0.780, 1.773]	0.912 [0.841, 0.958]	1.346 [1.159, 1.	0.836 [0.722, 0.926]
y75vj	Direct scheme for type III submission	1.901 [1.504, 2.270]	1.584 [1.221, 1.974]	1.039 [0.472, 1.614]	0.891 [0.791, 0.952]	1.345 [1.162, 1.	0.746 [0.564, 0.882]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.221, 2.713]	1.435 [1.043, 1.935]	-0.467 [-1.084, 0.260]	0.709 [0.601, 0.869]	1.083 [0.801, 1.	0.752 [0.615, 0.859]
w4iyd	Vertical scheme for type III submission	1.939 [1.527, 2.299]	1.578 [1.178, 1.981]	1.211 [0.653, 1.745]	0.849 [0.711, 0.928]	1.256 [1.009, 1.	0.715 [0.546, 0.837]
pwn3m	Analog_search	1.970 [0.760, 2.850]	1.115 [0.564, 1.786]	0.285 [-0.394, 1.092]	0.354 [0.015, 0.904]	0.583 [0.078, 1.	0.449 [0.113, 0.745]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.375, 2.941]	1.578 [1.098, 2.157]	-0.733 [-1.422, 0.036]	0.769 [0.671, 0.891]	1.291 [1.020, 1.	0.762 [0.631, 0.866]
xikp8	Direct scheme with single point correction for...	2.340 [1.911, 2.724]	2.026 [1.610, 2.448]	0.933 [0.132, 1.706]	0.867 [0.766, 0.931]	1.524 [1.294, 1.	0.737 [0.559, 0.877]
5nm4j	Substructure matches from experimental data	2.450 [1.412, 3.350]	1.583 [0.934, 2.348]	0.046 [-0.799, 1.030]	0.192 [0.002, 0.696]	0.398 [-0.059, 0	0.337 [-0.036, 0.667]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.597, 3.279]	1.744 [1.142, 2.407]	-0.526 [-1.351, 0.370]	0.726 [0.596, 0.850]	1.373 [1.034, 1.	0.758 [0.619, 0.867]
0hxtm	COSMOtherm_FINE17	2.638 [0.873, 3.799]	1.423 [0.660, 2.364]	0.736 [-0.145, 1.806]	0.127 [0.000, 0.841]	0.406 [-0.209, 1	0.367 [0.023, 0.703]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.453, 4.608]	1.883 [1.234, 2.836]	-0.230 [-1.414, 0.699]	0.540 [0.242, 0.882]	1.171 [0.960, 1.	0.606 [0.414, 0.773]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.279, 4.731]	1.695 [1.017, 2.740]	-0.773 [-1.929, 0.116]	0.516 [0.219, 0.884]	1.147 [0.952, 1.	0.575 [0.358, 0.751]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.457, 4.616]	1.841 [1.175, 2.788]	-0.491 [-1.597, 0.404]	0.547 [0.253, 0.872]	1.192 [0.984, 1.	0.577 [0.395, 0.737]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.492, 5.078]	1.985 [1.240, 3.066]	-0.102 [-1.393, 0.961]	0.523 [0.230, 0.872]	1.296 [1.033, 1.	0.617 [0.408, 0.790]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.491, 5.071]	1.997 [1.238, 3.067]	-0.138 [-1.415, 0.911]	0.526 [0.238, 0.872]	1.305 [1.038, 1.	0.617 [0.409, 0.790]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.883, 6.406]	2.443 [1.512, 3.785]	-0.470 [-2.069, 0.794]	0.486 [0.193, 0.878]	1.435 [1.132, 1.	0.626 [0.419, 0.788]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.442, 6.865]	2.999 [1.999, 4.408]	-0.370 [-2.138, 1.106]	0.517 [0.223, 0.880]	1.642 [1.312, 1.	0.612 [0.408, 0.783]

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.