ID τ	name	RMSE	MAE	ME	R^2	m
xvxzd 0.816 [0.680, 0.918]	Full quantum chemical calculation of free ener...	0.680 [0.543, 0.809]	0.579 [0.450, 0.711]	0.235 [-0.010, 0.455]	0.937 [0.876, 0.972]	0.923 [0.839, 1.
gyuhx 0.878 [0.803, 0.942]	S+pKa	0.732 [0.554, 0.906]	0.585 [0.439, 0.743]	0.035 [-0.234, 0.283]	0.929 [0.877, 0.965]	0.979 [0.903, 1.
xmyhm 0.807 [0.684, 0.901]	ACD/pKa Classic	0.787 [0.521, 1.033]	0.564 [0.383, 0.768]	0.134 [-0.145, 0.411]	0.919 [0.847, 0.968]	0.961 [0.859, 1.
nb017 0.726 [0.596, 0.835]	MoKa	0.943 [0.722, 1.159]	0.770 [0.585, 0.975]	-0.162 [-0.492, 0.164]	0.884 [0.808, 0.937]	0.939 [0.824, 1.
nb007 0.787 [0.652, 0.891]	Epik Scan	0.946 [0.733, 1.152]	0.776 [0.595, 0.968]	0.045 [-0.287, 0.372]	0.879 [0.765, 0.946]	0.840 [0.767, 0.
yqkga 0.827 [0.720, 0.908]	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.778, 1.232]	0.799 [0.588, 1.030]	-0.166 [-0.507, 0.186]	0.867 [0.782, 0.935]	0.927 [0.766, 1.
nb010 0.800 [0.670, 0.899]	Epik Microscopic	1.028 [0.770, 1.263]	0.814 [0.606, 1.040]	0.243 [-0.115, 0.585]	0.869 [0.768, 0.938]	0.946 [0.826, 1.
8xt50 0.801 [0.684, 0.893]	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.783, 1.360]	0.814 [0.584, 1.073]	-0.475 [-0.816, -0.138]	0.906 [0.842, 0.951]	1.078 [0.936, 1.
nb013 0.792 [0.638, 0.902]	Jaguar	1.103 [0.715, 1.470]	0.803 [0.562, 1.088]	-0.148 [-0.546, 0.220]	0.884 [0.782, 0.946]	1.092 [0.903, 1.
nb015 0.775 [0.662, 0.862]	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.982, 1.564]	1.044 [0.795, 1.307]	0.129 [-0.324, 0.557]	0.874 [0.797, 0.933]	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 [0.509, 1.000]	1.185 [0.355, 1.
37xm8 0.704 [0.562, 0.827]	ACD/pKa GALAS	1.413 [0.930, 1.840]	1.008 [0.678, 1.384]	-0.183 [-0.688, 0.316]	0.834 [0.698, 0.927]	1.155 [0.977, 1.
mkhqa 0.637 [0.444, 0.789]	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.129, 2.048]	1.239 [0.904, 1.616]	-0.316 [-0.885, 0.209]	0.803 [0.666, 0.906]	1.140 [0.976, 1.
ttjd0 0.650 [0.466, 0.798]	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.197, 2.064]	1.296 [0.956, 1.667]	-0.122 [-0.699, 0.449]	0.813 [0.686, 0.908]	1.198 [1.030, 1.
nb001 0.723 [0.549, 0.848]	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.053, 2.374]	1.213 [0.844, 1.676]	0.442 [-0.102, 1.035]	0.797 [0.700, 0.898]	1.156 [0.952, 1.
nb002 0.723 [0.556, 0.842]	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.082, 2.378]	1.246 [0.888, 1.700]	0.509 [-0.039, 1.101]	0.796 [0.698, 0.898]	1.153 [0.950, 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 [0.457, 1.000]	1.446 [0.735, 2.
ryzue 0.822 [0.712, 0.911]	Adiabatic scheme with single point correction ...	1.774 [1.422, 2.116]	1.500 [1.171, 1.844]	1.298 [0.859, 1.724]	0.910 [0.862, 0.949]	1.229 [1.057, 1.
2ii2g 0.680 [0.497, 0.820]	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.308, 2.241]	1.389 [1.010, 1.815]	-0.744 [-1.291, -0.149]	0.792 [0.653, 0.894]	1.149 [0.963, 1.
mpwiy 0.659 [0.491, 0.795]	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.392, 2.235]	1.482 [1.137, 1.877]	0.103 [-0.543, 0.731]	0.820 [0.702, 0.906]	1.294 [1.121, 1.
5byn6 0.830 [0.723, 0.917]	Adiabatic scheme for type III submission	1.890 [1.497, 2.267]	1.588 [1.238, 1.966]	1.317 [0.841, 1.799]	0.905 [0.849, 0.948]	1.284 [1.103, 1.

Continued on next page

ID	name	RMSE	MAE	ME	R^2	m	τ
y75vj	Direct scheme for type III submission	1.901 [1.496, 2.259]	1.584 [1.211, 1.973]	1.039 [0.463, 1.602]	0.891 [0.790, 0.952]	1.345 [1.161, 1.	0.746 [0.567, 0.879]
w4iyd	Vertical scheme for type III submission	1.926 [1.528, 2.280]	1.584 [1.203, 1.979]	1.257 [0.723, 1.764]	0.853 [0.742, 0.922]	1.206 [0.996, 1.	0.729 [0.571, 0.845]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.209, 2.707]	1.435 [1.036, 1.938]	-0.467 [-1.076, 0.244]	0.709 [0.603, 0.870]	1.083 [0.813, 1.	0.752 [0.616, 0.859]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.377, 2.628]	1.568 [1.165, 2.038]	0.557 [-0.098, 1.273]	0.823 [0.724, 0.903]	1.350 [1.146, 1.	0.715 [0.543, 0.843]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.392, 2.645]	1.577 [1.178, 2.040]	0.524 [-0.138, 1.223]	0.825 [0.728, 0.906]	1.358 [1.155, 1.	0.715 [0.538, 0.844]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.725, 2.332]	1.805 [1.476, 2.135]	-0.405 [-1.086, 0.312]	0.469 [0.284, 0.641]	0.559 [0.346, 0.	0.532 [0.350, 0.681]
hytjn	OE Gaussian Process	2.161 [1.244, 3.059]	1.389 [0.857, 2.039]	0.709 [0.028, 1.481]	0.449 [0.129, 0.784]	0.621 [0.259, 1.	0.472 [0.161, 0.734]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.380, 2.954]	1.578 [1.089, 2.155]	-0.733 [-1.422, 0.038]	0.769 [0.668, 0.892]	1.291 [1.015, 1.	0.762 [0.631, 0.864]
q3pfp	OE Gaussian Process Resampled	2.193 [1.332, 3.089]	1.505 [0.993, 2.126]	0.589 [-0.102, 1.372]	0.443 [0.127, 0.766]	0.658 [0.273, 1.	0.502 [0.198, 0.752]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.616, 2.805]	1.778 [1.343, 2.271]	0.784 [0.064, 1.519]	0.822 [0.696, 0.905]	1.406 [1.200, 1.	0.722 [0.549, 0.847]
xikp8	Direct scheme with single point correction for...	2.348 [1.936, 2.725]	2.056 [1.658, 2.475]	0.773 [-0.022, 1.581]	0.890 [0.797, 0.947]	1.588 [1.395, 1.	0.759 [0.589, 0.891]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.788, 2.946]	1.915 [1.444, 2.426]	0.313 [-0.488, 1.148]	0.842 [0.744, 0.914]	1.557 [1.341, 1.	0.715 [0.545, 0.834]
5nm4j	Substructure matches from experimental data	2.450 [1.415, 3.344]	1.583 [0.940, 2.344]	0.046 [-0.799, 1.070]	0.192 [0.002, 0.703]	0.398 [-0.062, 0	0.337 [-0.040, 0.666]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.675, 3.300]	1.826 [1.244, 2.486]	-0.651 [-1.477, 0.253]	0.761 [0.635, 0.876]	1.432 [1.120, 1.	0.774 [0.633, 0.880]
pwn3m	Analog_search	2.604 [1.450, 3.535]	1.539 [0.835, 2.371]	0.788 [-0.056, 1.766]	0.208 [0.005, 0.634]	0.369 [0.008, 0.	0.344 [0.041, 0.631]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.374, 3.564]	2.525 [2.001, 3.099]	0.424 [-0.601, 1.472]	0.844 [0.740, 0.916]	1.784 [1.551, 2.	0.715 [0.541, 0.843]
0hxtm	COSMOtherm_FINE17	3.263 [1.814, 4.389]	1.918 [1.026, 2.980]	1.377 [0.368, 2.561]	0.075 [0.000, 0.477]	0.281 [-0.175, 0	0.286 [-0.041, 0.607]

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.