ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.547, 0.810]	0.579 [0.453, 0.712]	0.235 [-0.002, 0.461]	0.937 [0.879, 0.972]	0.923 [0.836, 1.015]
gyuhx	S+pKa	0.732 [0.554, 0.910]	0.585 [0.435, 0.746]	0.035 [-0.230, 0.283]	0.929 [0.878, 0.965]	0.979 [0.903, 1.086]
xmyhm	ACD/pKa Classic	0.787 [0.526, 1.033]	0.564 [0.385, 0.767]	0.134 [-0.135, 0.401]	0.919 [0.847, 0.967]	0.961 [0.860, 1.078]
nb007	Epik-sequential	0.968 [0.765, 1.172]	0.810 [0.632, 1.001]	0.025 [-0.330, 0.352]	0.871 [0.763, 0.935]	0.874 [0.789, 0.977]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.772, 1.225]	0.799 [0.582, 1.019]	-0.166 [-0.495, 0.200]	0.867 [0.783, 0.935]	0.927 [0.768, 1.080]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.783, 1.355]	0.814 [0.578, 1.067]	-0.475 [-0.816, -0.141]	0.906 [0.841, 0.952]	1.078 [0.935, 1.219]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.428, 1.720]	-0.924 [-1.704, -0.108]	0.910 [0.509, 1.000]	1.185 [0.339, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.924, 1.843]	1.008 [0.672, 1.377]	-0.183 [-0.690, 0.322]	0.834 [0.698, 0.927]	1.155 [0.979, 1.332]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.134, 2.047]	1.239 [0.901, 1.613]	-0.316 [-0.883, 0.220]	0.803 [0.674, 0.906]	1.140 [0.982, 1.336]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.198, 2.073]	1.296 [0.956, 1.676]	-0.122 [-0.714, 0.447]	0.813 [0.680, 0.909]	1.198 [1.021, 1.399]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.057, 2.357]	1.213 [0.852, 1.670]	0.442 [-0.094, 1.048]	0.797 [0.697, 0.900]	1.156 [0.959, 1.425]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.081, 2.390]	1.246 [0.885, 1.701]	0.509 [-0.040, 1.102]	0.796 [0.699, 0.897]	1.153 [0.947, 1.429]
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]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.421, 2.115]	1.500 [1.177, 1.835]	1.298 [0.869, 1.722]	0.910 [0.861, 0.948]	1.229 [1.059, 1.405]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.309, 2.243]	1.389 [1.017, 1.806]	-0.744 [-1.303, -0.169]	0.792 [0.655, 0.893]	1.149 [0.962, 1.377]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.387, 2.222]	1.482 [1.129, 1.862]	0.103 [-0.572, 0.735]	0.820 [0.700, 0.906]	1.294 [1.116, 1.502]
5byn6	Adiabatic scheme for type III submission	1.890 [1.498, 2.260]	1.588 [1.235, 1.957]	1.317 [0.828, 1.800]	0.905 [0.850, 0.947]	1.284 [1.110, 1.468]
y75vj	Direct scheme for type III submission	1.901 [1.496, 2.256]	1.584 [1.212, 1.964]	1.039 [0.472, 1.604]	0.891 [0.792, 0.950]	1.345 [1.155, 1.528]
w4iyd	Vertical scheme for type III submission	1.926 [1.528, 2.283]	1.584 [1.202, 1.978]	1.257 [0.744, 1.776]	0.853 [0.737, 0.922]	1.206 [0.999, 1.399]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.223, 2.725]	1.435 [1.037, 1.945]	-0.467 [-1.095, 0.266]	0.709 [0.603, 0.867]	1.083 [0.809, 1.435]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.372, 2.657]	1.568 [1.163, 2.054]	0.557 [-0.107, 1.264]	0.823 [0.723, 0.903]	1.350 [1.147, 1.605]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.374, 2.648]	1.577 [1.167, 2.047]	0.524 [-0.140, 1.235]	0.825 [0.726, 0.905]	1.358 [1.151, 1.605]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.715, 2.328]	1.805 [1.470, 2.136]	-0.405 [-1.089, 0.325]	0.469 [0.291, 0.646]	0.559 [0.348, 0.836]
hytjn	OE Gaussian Process	2.161 [1.245, 3.078]	1.389 [0.861, 2.045]	0.709 [0.020, 1.487]	0.449 [0.128, 0.783]	0.621 [0.257, 1.003]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.377, 2.957]	1.578 [1.081, 2.155]	-0.733 [-1.426, 0.041]	0.769 [0.666, 0.890]	1.291 [1.016, 1.633]
q3pfp	OE Gaussian Process Resampled	2.193 [1.325, 3.077]	1.505 [0.991, 2.129]	0.589 [-0.101, 1.392]	0.443 [0.131, 0.765]	0.658 [0.278, 1.060]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.620, 2.821]	1.778 [1.345, 2.280]	0.784 [0.062, 1.526]	0.822 [0.698, 0.906]	1.406 [1.202, 1.629]
xikp8	Direct scheme with single point correction for...	2.348 [1.942, 2.727]	2.056 [1.660, 2.468]	0.773 [-0.051, 1.570]	0.890 [0.797, 0.947]	1.588 [1.394, 1.803]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.779, 2.951]	1.915 [1.430, 2.433]	0.313 [-0.501, 1.146]	0.842 [0.740, 0.912]	1.557 [1.342, 1.822]
5nm4j	Substructure matches from experimental data	2.450 [1.427, 3.338]	1.583 [0.944, 2.341]	0.046 [-0.815, 1.024]	0.192 [0.002, 0.687]	0.398 [-0.055, 0.812]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.692, 3.302]	1.826 [1.261, 2.494]	-0.651 [-1.493, 0.224]	0.761 [0.632, 0.876]	1.432 [1.127, 1.781]
pwn3m	Analog_search	2.604 [1.457, 3.498]	1.539 [0.826, 2.346]	0.788 [-0.051, 1.745]	0.208 [0.004, 0.628]	0.369 [0.009, 0.772]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.380, 3.557]	2.525 [1.991, 3.090]	0.424 [-0.606, 1.438]	0.844 [0.743, 0.916]	1.784 [1.554, 2.054]
0hxtm	COSMOtherm_FINE17	3.263 [1.822, 4.369]	1.918 [1.020, 2.962]	1.377 [0.379, 2.540]	0.075 [0.000, 0.481]	0.281 [-0.178, 0.836]

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-sequencial method (submission ID: nb007) were not blind. They were submitted after the submission deadline to be used as a reference method.