ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.547, 0.811]	0.579 [0.454, 0.711]	0.235 [-0.007, 0.462]	0.937 [0.877, 0.972]	0.923 [0.839, 1.017]
gyuhx	S+pKa	0.732 [0.557, 0.915]	0.585 [0.438, 0.748]	0.035 [-0.227, 0.285]	0.929 [0.876, 0.965]	0.979 [0.903, 1.084]
xmyhm	ACD/pKa Classic	0.787 [0.521, 1.032]	0.564 [0.385, 0.770]	0.134 [-0.145, 0.401]	0.919 [0.846, 0.967]	0.961 [0.856, 1.081]
nb017	MoKa	0.943 [0.725, 1.152]	0.770 [0.586, 0.972]	-0.162 [-0.491, 0.163]	0.884 [0.806, 0.937]	0.939 [0.820, 1.075]
nb007	Epik Scan	0.946 [0.732, 1.158]	0.776 [0.593, 0.980]	0.045 [-0.298, 0.364]	0.879 [0.764, 0.944]	0.840 [0.767, 0.921]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.778, 1.229]	0.799 [0.587, 1.022]	-0.166 [-0.513, 0.195]	0.867 [0.782, 0.933]	0.927 [0.764, 1.076]
nb010	Epik Microscopic	1.028 [0.771, 1.262]	0.814 [0.606, 1.039]	0.243 [-0.116, 0.582]	0.869 [0.773, 0.939]	0.946 [0.828, 1.078]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.783, 1.361]	0.814 [0.577, 1.070]	-0.475 [-0.824, -0.142]	0.906 [0.841, 0.951]	1.078 [0.936, 1.219]
nb013	Jaguar	1.103 [0.715, 1.479]	0.803 [0.563, 1.087]	-0.148 [-0.555, 0.211]	0.884 [0.782, 0.946]	1.092 [0.907, 1.255]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.980, 1.568]	1.044 [0.792, 1.308]	0.129 [-0.330, 0.560]	0.874 [0.797, 0.932]	1.162 [0.937, 1.342]
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 [0.509, 1.000]	1.185 [0.339, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.931, 1.850]	1.008 [0.682, 1.386]	-0.183 [-0.678, 0.321]	0.834 [0.693, 0.927]	1.155 [0.978, 1.335]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.146, 2.046]	1.239 [0.916, 1.613]	-0.316 [-0.872, 0.221]	0.803 [0.666, 0.902]	1.140 [0.981, 1.342]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.200, 2.064]	1.296 [0.955, 1.671]	-0.122 [-0.722, 0.436]	0.813 [0.687, 0.907]	1.198 [1.028, 1.405]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.057, 2.380]	1.213 [0.845, 1.671]	0.442 [-0.092, 1.053]	0.797 [0.699, 0.899]	1.156 [0.954, 1.430]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.083, 2.390]	1.246 [0.890, 1.701]	0.509 [-0.031, 1.118]	0.796 [0.699, 0.896]	1.153 [0.949, 1.421]
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 [0.463, 1.000]	1.446 [0.735, 2.147]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.416, 2.118]	1.500 [1.171, 1.843]	1.298 [0.860, 1.708]	0.910 [0.860, 0.949]	1.229 [1.060, 1.406]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.309, 2.255]	1.389 [1.009, 1.809]	-0.744 [-1.307, -0.160]	0.792 [0.652, 0.892]	1.149 [0.959, 1.370]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.390, 2.219]	1.482 [1.127, 1.861]	0.103 [-0.552, 0.737]	0.820 [0.705, 0.906]	1.294 [1.116, 1.507]
5byn6	Adiabatic scheme for type III submission	1.890 [1.507, 2.259]	1.588 [1.245, 1.958]	1.317 [0.837, 1.778]	0.905 [0.850, 0.948]	1.284 [1.106, 1.471]
y75vj	Direct scheme for type III submission	1.901 [1.507, 2.269]	1.584 [1.226, 1.968]	1.039 [0.476, 1.615]	0.891 [0.792, 0.951]	1.345 [1.161, 1.529]
w4iyd	Vertical scheme for type III submission	1.926 [1.531, 2.279]	1.584 [1.205, 1.976]	1.257 [0.724, 1.760]	0.853 [0.737, 0.922]	1.206 [0.998, 1.403]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.213, 2.715]	1.435 [1.035, 1.945]	-0.467 [-1.072, 0.252]	0.709 [0.601, 0.872]	1.083 [0.807, 1.440]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.374, 2.640]	1.568 [1.160, 2.044]	0.557 [-0.087, 1.258]	0.823 [0.723, 0.902]	1.350 [1.153, 1.605]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.384, 2.629]	1.577 [1.176, 2.045]	0.524 [-0.139, 1.224]	0.825 [0.724, 0.906]	1.358 [1.156, 1.610]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.714, 2.325]	1.805 [1.465, 2.134]	-0.405 [-1.070, 0.324]	0.469 [0.289, 0.644]	0.559 [0.348, 0.824]
hytjn	OE Gaussian Process	2.161 [1.247, 3.083]	1.389 [0.855, 2.042]	0.709 [0.020, 1.483]	0.449 [0.124, 0.784]	0.621 [0.248, 1.003]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.378, 2.918]	1.578 [1.091, 2.135]	-0.733 [-1.427, 0.036]	0.769 [0.667, 0.892]	1.291 [1.017, 1.626]
q3pfp	OE Gaussian Process Resampled	2.193 [1.341, 3.099]	1.505 [1.004, 2.138]	0.589 [-0.107, 1.397]	0.443 [0.138, 0.767]	0.658 [0.283, 1.067]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.604, 2.820]	1.778 [1.334, 2.276]	0.784 [0.076, 1.531]	0.822 [0.697, 0.905]	1.406 [1.197, 1.627]
xikp8	Direct scheme with single point correction for...	2.348 [1.940, 2.729]	2.056 [1.662, 2.470]	0.773 [-0.014, 1.552]	0.890 [0.796, 0.946]	1.588 [1.395, 1.805]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.796, 2.945]	1.915 [1.437, 2.422]	0.313 [-0.496, 1.158]	0.842 [0.741, 0.912]	1.557 [1.341, 1.819]
5nm4j	Substructure matches from experimental data	2.450 [1.410, 3.351]	1.583 [0.926, 2.339]	0.046 [-0.815, 1.035]	0.192 [0.002, 0.698]	0.398 [-0.067, 0.822]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.684, 3.307]	1.826 [1.262, 2.485]	-0.651 [-1.501, 0.264]	0.761 [0.627, 0.875]	1.432 [1.136, 1.774]
pwn3m	Analog_search	2.604 [1.459, 3.518]	1.539 [0.832, 2.366]	0.788 [-0.058, 1.756]	0.208 [0.003, 0.635]	0.369 [-0.001, 0.779]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.356, 3.574]	2.525 [1.975, 3.105]	0.424 [-0.595, 1.472]	0.844 [0.738, 0.917]	1.784 [1.547, 2.058]
0hxtm	COSMOtherm_FINE17	3.263 [1.777, 4.396]	1.918 [1.014, 2.968]	1.377 [0.349, 2.570]	0.075 [0.000, 0.497]	0.281 [-0.174, 0.844]

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.