ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.544, 0.811]	0.579 [0.449, 0.714]	0.235 [-0.007, 0.464]	0.937 [0.878, 0.973]	0.923 [0.837, 1.016]
gyuhx	S+pKa	0.732 [0.554, 0.910]	0.585 [0.437, 0.744]	0.035 [-0.229, 0.283]	0.929 [0.878, 0.966]	0.979 [0.904, 1.086]
xmyhm	ACD/pKa Classic	0.787 [0.519, 1.032]	0.564 [0.383, 0.772]	0.134 [-0.145, 0.406]	0.919 [0.847, 0.968]	0.961 [0.855, 1.085]
nb017	MoKa	0.943 [0.723, 1.154]	0.770 [0.586, 0.969]	-0.162 [-0.497, 0.160]	0.884 [0.808, 0.937]	0.939 [0.821, 1.076]
nb007	Epik Scan	0.946 [0.734, 1.159]	0.776 [0.597, 0.975]	0.045 [-0.288, 0.369]	0.879 [0.764, 0.946]	0.840 [0.766, 0.922]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.779, 1.227]	0.799 [0.588, 1.020]	-0.166 [-0.511, 0.192]	0.867 [0.780, 0.935]	0.927 [0.763, 1.084]
nb010	Epik Microscopic	1.028 [0.769, 1.276]	0.814 [0.601, 1.049]	0.243 [-0.113, 0.593]	0.869 [0.770, 0.940]	0.946 [0.827, 1.080]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.786, 1.355]	0.814 [0.584, 1.065]	-0.475 [-0.821, -0.146]	0.906 [0.841, 0.952]	1.078 [0.929, 1.218]
nb013	Jaguar	1.103 [0.710, 1.473]	0.803 [0.559, 1.091]	-0.148 [-0.548, 0.214]	0.884 [0.782, 0.948]	1.092 [0.905, 1.257]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.991, 1.567]	1.044 [0.803, 1.305]	0.129 [-0.335, 0.562]	0.874 [0.799, 0.933]	1.162 [0.934, 1.336]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.448, 1.720]	-0.924 [-1.720, -0.108]	0.910 [0.509, 1.000]	1.185 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.936, 1.849]	1.008 [0.681, 1.378]	-0.183 [-0.682, 0.326]	0.834 [0.693, 0.926]	1.155 [0.979, 1.333]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.139, 2.043]	1.239 [0.912, 1.620]	-0.316 [-0.891, 0.215]	0.803 [0.668, 0.906]	1.140 [0.976, 1.339]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.201, 2.061]	1.296 [0.956, 1.667]	-0.122 [-0.693, 0.442]	0.813 [0.688, 0.908]	1.198 [1.029, 1.394]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.059, 2.382]	1.213 [0.851, 1.668]	0.442 [-0.100, 1.046]	0.797 [0.699, 0.896]	1.156 [0.955, 1.429]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.071, 2.377]	1.246 [0.879, 1.695]	0.509 [-0.036, 1.112]	0.796 [0.700, 0.896]	1.153 [0.951, 1.427]
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 [0.720, 2.130]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.408, 2.117]	1.500 [1.172, 1.843]	1.298 [0.862, 1.724]	0.910 [0.863, 0.948]	1.229 [1.060, 1.401]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.297, 2.254]	1.389 [1.005, 1.816]	-0.744 [-1.307, -0.170]	0.792 [0.655, 0.892]	1.149 [0.961, 1.375]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.382, 2.218]	1.482 [1.125, 1.869]	0.103 [-0.561, 0.717]	0.820 [0.705, 0.906]	1.294 [1.116, 1.505]
5byn6	Adiabatic scheme for type III submission	1.890 [1.512, 2.262]	1.588 [1.238, 1.955]	1.317 [0.828, 1.791]	0.905 [0.848, 0.947]	1.284 [1.107, 1.471]
y75vj	Direct scheme for type III submission	1.901 [1.508, 2.259]	1.584 [1.225, 1.962]	1.039 [0.473, 1.600]	0.891 [0.794, 0.952]	1.345 [1.161, 1.528]
w4iyd	Vertical scheme for type III submission	1.926 [1.516, 2.284]	1.584 [1.190, 1.975]	1.257 [0.729, 1.767]	0.853 [0.738, 0.922]	1.206 [0.998, 1.401]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.219, 2.724]	1.435 [1.038, 1.950]	-0.467 [-1.069, 0.231]	0.709 [0.604, 0.868]	1.083 [0.809, 1.448]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.379, 2.646]	1.568 [1.166, 2.051]	0.557 [-0.082, 1.264]	0.823 [0.725, 0.902]	1.350 [1.149, 1.607]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.387, 2.660]	1.577 [1.172, 2.049]	0.524 [-0.131, 1.242]	0.825 [0.726, 0.903]	1.358 [1.154, 1.607]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.730, 2.323]	1.805 [1.477, 2.135]	-0.405 [-1.095, 0.319]	0.469 [0.283, 0.643]	0.559 [0.346, 0.825]
hytjn	OE Gaussian Process	2.161 [1.243, 3.049]	1.389 [0.858, 2.031]	0.709 [0.016, 1.483]	0.449 [0.129, 0.783]	0.621 [0.257, 0.997]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.384, 2.955]	1.578 [1.099, 2.153]	-0.733 [-1.414, 0.039]	0.769 [0.665, 0.891]	1.291 [1.023, 1.642]
q3pfp	OE Gaussian Process Resampled	2.193 [1.330, 3.086]	1.505 [0.997, 2.129]	0.589 [-0.117, 1.403]	0.443 [0.124, 0.766]	0.658 [0.269, 1.068]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.615, 2.835]	1.778 [1.332, 2.289]	0.784 [0.064, 1.538]	0.822 [0.695, 0.905]	1.406 [1.198, 1.627]
xikp8	Direct scheme with single point correction for...	2.348 [1.937, 2.722]	2.056 [1.654, 2.472]	0.773 [-0.042, 1.575]	0.890 [0.799, 0.947]	1.588 [1.392, 1.804]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.803, 2.941]	1.915 [1.452, 2.432]	0.313 [-0.484, 1.156]	0.842 [0.739, 0.912]	1.557 [1.346, 1.818]
5nm4j	Substructure matches from experimental data	2.450 [1.418, 3.329]	1.583 [0.943, 2.348]	0.046 [-0.824, 1.015]	0.192 [0.002, 0.696]	0.398 [-0.064, 0.815]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.674, 3.294]	1.826 [1.245, 2.476]	-0.651 [-1.507, 0.230]	0.761 [0.634, 0.875]	1.432 [1.125, 1.765]
pwn3m	Analog_search	2.604 [1.446, 3.497]	1.539 [0.823, 2.350]	0.788 [-0.071, 1.725]	0.208 [0.003, 0.635]	0.369 [0.003, 0.782]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.366, 3.575]	2.525 [1.979, 3.115]	0.424 [-0.606, 1.466]	0.844 [0.738, 0.915]	1.784 [1.554, 2.055]
0hxtm	COSMOtherm_FINE17	3.263 [1.788, 4.386]	1.918 [1.003, 2.966]	1.377 [0.346, 2.546]	0.075 [0.000, 0.477]	0.281 [-0.171, 0.839]

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.