ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.547, 0.815]	0.579 [0.451, 0.714]	0.235 [-0.007, 0.460]	0.937 [0.879, 0.972]	0.923 [0.837, 1.017]
gyuhx	S+pKa	0.730 [0.547, 0.914]	0.579 [0.425, 0.743]	0.009 [-0.257, 0.262]	0.925 [0.869, 0.963]	0.996 [0.913, 1.109]
xmyhm	ACD/pKa Classic	0.774 [0.495, 1.031]	0.546 [0.363, 0.761]	0.102 [-0.177, 0.375]	0.916 [0.826, 0.968]	0.981 [0.872, 1.107]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.684, 1.126]	0.710 [0.518, 0.923]	-0.288 [-0.578, 0.035]	0.901 [0.821, 0.953]	1.000 [0.864, 1.128]
nb017	MoKa	0.943 [0.733, 1.151]	0.770 [0.592, 0.966]	-0.162 [-0.496, 0.163]	0.884 [0.805, 0.937]	0.939 [0.819, 1.076]
nb007	Epik Scan	0.946 [0.730, 1.156]	0.776 [0.593, 0.973]	0.045 [-0.293, 0.375]	0.879 [0.763, 0.945]	0.840 [0.767, 0.923]
nb010	Epik Microscopic	1.028 [0.774, 1.274]	0.814 [0.604, 1.048]	0.243 [-0.119, 0.585]	0.869 [0.766, 0.939]	0.946 [0.827, 1.076]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.786, 1.362]	0.814 [0.583, 1.072]	-0.475 [-0.818, -0.143]	0.906 [0.840, 0.950]	1.078 [0.936, 1.217]
nb013	Jaguar	1.103 [0.709, 1.470]	0.803 [0.558, 1.090]	-0.148 [-0.546, 0.210]	0.884 [0.784, 0.947]	1.092 [0.902, 1.250]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.986, 1.564]	1.044 [0.798, 1.307]	0.129 [-0.326, 0.559]	0.874 [0.797, 0.933]	1.162 [0.943, 1.337]
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 [0.522, 1.000]	1.185 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.852, 1.807]	0.955 [0.641, 1.331]	-0.101 [-0.573, 0.395]	0.854 [0.731, 0.939]	1.171 [1.001, 1.359]
hytjn	OE Gaussian Process	1.434 [0.985, 1.835]	1.034 [0.686, 1.425]	0.240 [-0.271, 0.776]	0.675 [0.420, 0.853]	0.849 [0.556, 1.095]
q3pfp	OE Gaussian Process Resampled	1.484 [1.050, 1.874]	1.140 [0.806, 1.513]	0.090 [-0.446, 0.669]	0.667 [0.425, 0.839]	0.886 [0.579, 1.171]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.133, 2.039]	1.239 [0.904, 1.612]	-0.316 [-0.878, 0.220]	0.803 [0.669, 0.902]	1.140 [0.978, 1.336]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.206, 2.140]	1.304 [0.952, 1.698]	-1.061 [-1.543, -0.615]	0.837 [0.729, 0.915]	1.073 [0.930, 1.250]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.063, 2.389]	1.219 [0.846, 1.683]	0.422 [-0.122, 1.034]	0.792 [0.688, 0.899]	1.192 [0.970, 1.486]
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]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.078, 2.414]	1.250 [0.877, 1.723]	0.467 [-0.091, 1.102]	0.794 [0.688, 0.900]	1.200 [0.977, 1.496]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.363, 2.111]	1.436 [1.090, 1.806]	1.227 [0.785, 1.672]	0.922 [0.861, 0.963]	1.299 [1.124, 1.465]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.591, 2.153]	1.674 [1.364, 1.981]	-0.688 [-1.308, -0.027]	0.531 [0.328, 0.726]	0.670 [0.431, 0.982]
5byn6	Adiabatic scheme for type III submission	1.891 [1.492, 2.274]	1.553 [1.184, 1.938]	1.273 [0.770, 1.771]	0.912 [0.839, 0.959]	1.346 [1.162, 1.524]
y75vj	Direct scheme for type III submission	1.901 [1.504, 2.253]	1.584 [1.218, 1.958]	1.039 [0.465, 1.602]	0.891 [0.792, 0.950]	1.345 [1.165, 1.532]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.217, 2.721]	1.435 [1.042, 1.953]	-0.467 [-1.071, 0.260]	0.709 [0.603, 0.869]	1.083 [0.809, 1.444]
w4iyd	Vertical scheme for type III submission	1.939 [1.528, 2.306]	1.578 [1.181, 1.987]	1.211 [0.651, 1.747]	0.849 [0.715, 0.928]	1.256 [1.018, 1.458]
pwn3m	Analog_search	1.970 [0.774, 2.855]	1.115 [0.572, 1.809]	0.285 [-0.380, 1.100]	0.354 [0.013, 0.898]	0.583 [0.072, 1.034]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.365, 2.938]	1.578 [1.084, 2.138]	-0.733 [-1.412, 0.036]	0.769 [0.670, 0.891]	1.291 [1.013, 1.639]
xikp8	Direct scheme with single point correction for...	2.340 [1.907, 2.733]	2.026 [1.607, 2.456]	0.933 [0.126, 1.695]	0.867 [0.768, 0.931]	1.524 [1.294, 1.785]
5nm4j	Substructure matches from experimental data	2.450 [1.403, 3.358]	1.583 [0.931, 2.355]	0.046 [-0.809, 1.036]	0.192 [0.002, 0.702]	0.398 [-0.086, 0.824]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.592, 3.302]	1.744 [1.149, 2.437]	-0.526 [-1.354, 0.373]	0.726 [0.597, 0.852]	1.373 [1.044, 1.776]
0hxtm	COSMOtherm_FINE17	2.638 [0.879, 3.844]	1.423 [0.667, 2.406]	0.736 [-0.139, 1.838]	0.127 [0.000, 0.833]	0.406 [-0.223, 1.051]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.450, 4.603]	1.883 [1.243, 2.824]	-0.230 [-1.396, 0.697]	0.540 [0.239, 0.884]	1.171 [0.964, 1.376]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.294, 4.724]	1.695 [1.018, 2.728]	-0.773 [-1.962, 0.123]	0.516 [0.218, 0.882]	1.147 [0.949, 1.355]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.463, 4.640]	1.841 [1.176, 2.814]	-0.491 [-1.647, 0.413]	0.547 [0.247, 0.876]	1.192 [0.983, 1.420]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.498, 5.056]	1.985 [1.237, 3.067]	-0.102 [-1.379, 0.950]	0.523 [0.234, 0.871]	1.296 [1.028, 1.601]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.494, 5.057]	1.997 [1.242, 3.044]	-0.138 [-1.439, 0.918]	0.526 [0.235, 0.874]	1.305 [1.046, 1.606]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.877, 6.418]	2.443 [1.506, 3.831]	-0.470 [-2.142, 0.777]	0.486 [0.192, 0.877]	1.435 [1.125, 1.775]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.441, 6.882]	2.999 [2.002, 4.428]	-0.370 [-2.098, 1.120]	0.517 [0.227, 0.879]	1.642 [1.327, 1.986]

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.