ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.544, 0.807]	0.579 [0.452, 0.709]	-0.235 [-0.453, 0.007]	0.937 [0.877, 0.972]	1.015 [0.914, 1.117]
gyuhx	S+pKa	0.730 [0.549, 0.923]	0.579 [0.427, 0.750]	-0.009 [-0.260, 0.261]	0.925 [0.870, 0.963]	0.929 [0.813, 1.028]
xmyhm	ACD/pKa Classic	0.774 [0.491, 1.027]	0.546 [0.362, 0.756]	-0.102 [-0.373, 0.178]	0.916 [0.831, 0.969]	0.934 [0.816, 1.047]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.683, 1.122]	0.710 [0.518, 0.918]	0.288 [-0.025, 0.586]	0.901 [0.823, 0.953]	0.901 [0.773, 1.039]
nb007	Epik-sequential	0.968 [0.765, 1.166]	0.810 [0.631, 0.998]	-0.025 [-0.357, 0.321]	0.871 [0.765, 0.935]	0.997 [0.860, 1.120]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.784, 1.354]	0.814 [0.579, 1.064]	0.475 [0.148, 0.819]	0.906 [0.841, 0.952]	0.840 [0.745, 0.956]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.428, 1.720]	0.924 [0.108, 1.720]	0.910 [0.509, 1.000]	0.768 [0.558, 1.301]
37xm8	ACD/pKa GALAS	1.358 [0.851, 1.812]	0.955 [0.633, 1.332]	0.101 [-0.385, 0.595]	0.854 [0.730, 0.938]	0.729 [0.599, 0.878]
hytjn	OE Gaussian Process	1.434 [0.983, 1.834]	1.034 [0.683, 1.422]	-0.240 [-0.777, 0.274]	0.675 [0.416, 0.855]	0.795 [0.601, 1.001]
q3pfp	OE Gaussian Process Resampled	1.484 [1.058, 1.873]	1.140 [0.811, 1.512]	-0.090 [-0.658, 0.441]	0.667 [0.426, 0.836]	0.752 [0.565, 0.964]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.147, 2.052]	1.239 [0.911, 1.612]	0.316 [-0.223, 0.880]	0.803 [0.666, 0.902]	0.705 [0.567, 0.834]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.187, 2.144]	1.304 [0.938, 1.701]	1.061 [0.607, 1.533]	0.837 [0.728, 0.917]	0.780 [0.639, 0.927]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.069, 2.412]	1.219 [0.846, 1.685]	-0.422 [-1.036, 0.137]	0.792 [0.683, 0.898]	0.664 [0.512, 0.855]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	1.006 [-0.134, 2.178]	0.919 [0.457, 1.000]	0.635 [0.394, 0.806]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.072, 2.396]	1.250 [0.877, 1.714]	-0.467 [-1.075, 0.083]	0.794 [0.687, 0.902]	0.662 [0.517, 0.847]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.363, 2.112]	1.436 [1.089, 1.803]	-1.227 [-1.684, -0.780]	0.922 [0.862, 0.963]	0.710 [0.644, 0.799]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.587, 2.149]	1.674 [1.358, 1.980]	0.688 [0.027, 1.313]	0.531 [0.331, 0.724]	0.793 [0.575, 1.081]
5byn6	Adiabatic scheme for type III submission	1.891 [1.484, 2.281]	1.553 [1.177, 1.952]	-1.273 [-1.768, -0.761]	0.912 [0.840, 0.959]	0.677 [0.610, 0.760]
y75vj	Direct scheme for type III submission	1.901 [1.495, 2.262]	1.584 [1.216, 1.961]	-1.039 [-1.602, -0.465]	0.891 [0.792, 0.950]	0.663 [0.597, 0.737]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.205, 2.711]	1.435 [1.032, 1.946]	0.467 [-0.234, 1.090]	0.709 [0.602, 0.870]	0.655 [0.474, 0.972]
w4iyd	Vertical scheme for type III submission	1.939 [1.535, 2.304]	1.578 [1.185, 1.986]	-1.211 [-1.741, -0.669]	0.849 [0.723, 0.929]	0.676 [0.602, 0.773]
pwn3m	Analog_search	1.970 [0.766, 2.868]	1.115 [0.565, 1.808]	-0.285 [-1.106, 0.393]	0.354 [0.016, 0.900]	0.607 [0.137, 0.875]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.368, 2.946]	1.578 [1.093, 2.155]	0.733 [-0.054, 1.421]	0.769 [0.667, 0.894]	0.596 [0.456, 0.812]
xikp8	Direct scheme with single point correction for...	2.340 [1.915, 2.730]	2.026 [1.614, 2.453]	-0.933 [-1.694, -0.128]	0.867 [0.765, 0.932]	0.569 [0.492, 0.649]
5nm4j	Substructure matches from experimental data	2.450 [1.399, 3.331]	1.583 [0.918, 2.328]	-0.046 [-1.016, 0.794]	0.192 [0.002, 0.706]	0.484 [-0.075, 0.971]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.591, 3.322]	1.744 [1.139, 2.450]	0.526 [-0.369, 1.373]	0.726 [0.596, 0.850]	0.528 [0.408, 0.723]
0hxtm	COSMOtherm_FINE17	2.638 [0.885, 3.820]	1.423 [0.664, 2.379]	-0.736 [-1.816, 0.144]	0.127 [0.000, 0.839]	0.313 [-0.198, 0.777]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.443, 4.637]	1.883 [1.234, 2.869]	0.230 [-0.707, 1.410]	0.540 [0.242, 0.883]	0.461 [0.225, 0.749]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.276, 4.723]	1.695 [1.005, 2.723]	0.773 [-0.113, 1.936]	0.516 [0.221, 0.884]	0.450 [0.209, 0.777]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.454, 4.649]	1.841 [1.172, 2.812]	0.491 [-0.416, 1.665]	0.547 [0.244, 0.876]	0.459 [0.227, 0.743]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.487, 5.082]	1.985 [1.241, 3.072]	0.102 [-0.952, 1.438]	0.523 [0.223, 0.868]	0.404 [0.191, 0.701]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.500, 5.081]	1.997 [1.252, 3.070]	0.138 [-0.904, 1.428]	0.526 [0.236, 0.871]	0.403 [0.197, 0.697]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.902, 6.407]	2.443 [1.518, 3.801]	0.470 [-0.782, 2.068]	0.486 [0.196, 0.877]	0.339 [0.149, 0.625]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.444, 6.871]	2.999 [1.998, 4.406]	0.370 [-1.065, 2.140]	0.517 [0.221, 0.879]	0.315 [0.149, 0.542]

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.