ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.546, 0.809]	0.579 [0.453, 0.709]	-0.235 [-0.458, 0.009]	0.937 [0.878, 0.972]	1.015 [0.915, 1.115]
gyuhx	S+pKa	0.730 [0.545, 0.906]	0.579 [0.426, 0.739]	-0.009 [-0.260, 0.259]	0.925 [0.869, 0.964]	0.929 [0.812, 1.032]
xmyhm	ACD/pKa Classic	0.774 [0.493, 1.027]	0.546 [0.362, 0.753]	-0.102 [-0.373, 0.178]	0.916 [0.830, 0.969]	0.934 [0.819, 1.044]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.681, 1.120]	0.710 [0.512, 0.918]	0.288 [-0.034, 0.587]	0.901 [0.824, 0.953]	0.901 [0.774, 1.037]
nb007	Epik-sequential	0.968 [0.763, 1.174]	0.810 [0.628, 1.002]	-0.025 [-0.358, 0.319]	0.871 [0.764, 0.935]	0.997 [0.853, 1.117]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.782, 1.363]	0.814 [0.582, 1.076]	0.475 [0.145, 0.825]	0.906 [0.841, 0.951]	0.840 [0.745, 0.955]
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, 1.516]
37xm8	ACD/pKa GALAS	1.358 [0.848, 1.808]	0.955 [0.638, 1.334]	0.101 [-0.388, 0.610]	0.854 [0.730, 0.939]	0.729 [0.597, 0.878]
hytjn	OE Gaussian Process	1.434 [0.985, 1.818]	1.034 [0.684, 1.404]	-0.240 [-0.765, 0.272]	0.675 [0.415, 0.855]	0.795 [0.600, 1.005]
q3pfp	OE Gaussian Process Resampled	1.484 [1.060, 1.867]	1.140 [0.813, 1.505]	-0.090 [-0.642, 0.446]	0.667 [0.429, 0.835]	0.752 [0.567, 0.966]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.133, 2.035]	1.239 [0.902, 1.610]	0.316 [-0.221, 0.873]	0.803 [0.668, 0.904]	0.705 [0.567, 0.835]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.203, 2.133]	1.304 [0.947, 1.696]	1.061 [0.616, 1.532]	0.837 [0.731, 0.916]	0.780 [0.638, 0.929]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.060, 2.397]	1.219 [0.843, 1.688]	-0.422 [-1.036, 0.136]	0.792 [0.686, 0.900]	0.664 [0.514, 0.853]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.666, 2.338]	1.442 [0.624, 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 [1.081, 2.428]	1.250 [0.879, 1.731]	-0.467 [-1.108, 0.087]	0.794 [0.688, 0.899]	0.662 [0.517, 0.846]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.367, 2.102]	1.436 [1.093, 1.801]	-1.227 [-1.670, -0.781]	0.922 [0.862, 0.962]	0.710 [0.642, 0.799]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.592, 2.148]	1.674 [1.364, 1.977]	0.688 [0.022, 1.308]	0.531 [0.336, 0.725]	0.793 [0.575, 1.084]
5byn6	Adiabatic scheme for type III submission	1.891 [1.482, 2.275]	1.553 [1.177, 1.961]	-1.273 [-1.777, -0.768]	0.912 [0.843, 0.958]	0.677 [0.613, 0.759]
y75vj	Direct scheme for type III submission	1.901 [1.502, 2.260]	1.584 [1.220, 1.966]	-1.039 [-1.590, -0.474]	0.891 [0.791, 0.951]	0.663 [0.596, 0.735]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.206, 2.729]	1.435 [1.028, 1.950]	0.467 [-0.250, 1.076]	0.709 [0.603, 0.869]	0.655 [0.475, 0.972]
w4iyd	Vertical scheme for type III submission	1.939 [1.540, 2.307]	1.578 [1.190, 1.997]	-1.211 [-1.745, -0.657]	0.849 [0.711, 0.929]	0.676 [0.599, 0.772]
pwn3m	Analog_search	1.970 [0.760, 2.838]	1.115 [0.557, 1.792]	-0.285 [-1.082, 0.370]	0.354 [0.016, 0.902]	0.607 [0.137, 0.873]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.388, 2.943]	1.578 [1.096, 2.155]	0.733 [-0.042, 1.414]	0.769 [0.667, 0.889]	0.596 [0.455, 0.811]
xikp8	Direct scheme with single point correction for...	2.340 [1.904, 2.733]	2.026 [1.604, 2.458]	-0.933 [-1.718, -0.135]	0.867 [0.766, 0.931]	0.569 [0.491, 0.651]
5nm4j	Substructure matches from experimental data	2.450 [1.418, 3.358]	1.583 [0.939, 2.353]	-0.046 [-1.036, 0.790]	0.192 [0.002, 0.696]	0.484 [-0.089, 0.970]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.609, 3.309]	1.744 [1.148, 2.440]	0.526 [-0.391, 1.403]	0.726 [0.593, 0.851]	0.528 [0.405, 0.728]
0hxtm	COSMOtherm_FINE17	2.638 [0.869, 3.805]	1.423 [0.668, 2.366]	-0.736 [-1.789, 0.130]	0.127 [0.000, 0.835]	0.313 [-0.187, 0.780]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.446, 4.617]	1.883 [1.238, 2.831]	0.230 [-0.713, 1.403]	0.540 [0.242, 0.882]	0.461 [0.227, 0.749]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.271, 4.737]	1.695 [1.008, 2.735]	0.773 [-0.116, 1.925]	0.516 [0.219, 0.885]	0.450 [0.206, 0.774]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.456, 4.651]	1.841 [1.182, 2.833]	0.491 [-0.433, 1.660]	0.547 [0.253, 0.874]	0.459 [0.230, 0.741]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.496, 5.040]	1.985 [1.232, 3.056]	0.102 [-0.934, 1.376]	0.523 [0.230, 0.872]	0.404 [0.193, 0.702]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.500, 5.076]	1.997 [1.251, 3.067]	0.138 [-0.912, 1.392]	0.526 [0.238, 0.873]	0.403 [0.197, 0.694]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.889, 6.428]	2.443 [1.516, 3.851]	0.470 [-0.797, 2.136]	0.486 [0.190, 0.878]	0.339 [0.151, 0.626]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.445, 6.907]	2.999 [2.004, 4.441]	0.370 [-1.096, 2.162]	0.517 [0.219, 0.878]	0.315 [0.148, 0.540]

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.