ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.543, 0.809]	0.579 [0.451, 0.711]	0.235 [-0.005, 0.459]	0.937 [0.878, 0.972]	0.923 [0.838, 1.015]
gyuhx	S+pKa	0.730 [0.549, 0.914]	0.579 [0.427, 0.743]	0.009 [-0.253, 0.268]	0.925 [0.871, 0.964]	0.996 [0.910, 1.108]
xmyhm	ACD/pKa Classic	0.774 [0.498, 1.035]	0.546 [0.364, 0.758]	0.102 [-0.179, 0.374]	0.916 [0.831, 0.969]	0.981 [0.871, 1.106]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.683, 1.124]	0.710 [0.517, 0.922]	-0.288 [-0.581, 0.028]	0.901 [0.822, 0.953]	1.000 [0.868, 1.128]
nb007	Epik-sequential	0.968 [0.763, 1.175]	0.810 [0.627, 1.003]	0.025 [-0.319, 0.355]	0.871 [0.761, 0.935]	0.874 [0.786, 0.976]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.789, 1.358]	0.814 [0.585, 1.075]	-0.475 [-0.830, -0.137]	0.906 [0.840, 0.951]	1.078 [0.935, 1.216]
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 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.837, 1.812]	0.955 [0.635, 1.331]	-0.101 [-0.589, 0.389]	0.854 [0.724, 0.939]	1.171 [0.999, 1.346]
hytjn	OE Gaussian Process	1.434 [0.995, 1.829]	1.034 [0.688, 1.419]	0.240 [-0.277, 0.777]	0.675 [0.421, 0.854]	0.849 [0.550, 1.101]
q3pfp	OE Gaussian Process Resampled	1.484 [1.058, 1.867]	1.140 [0.805, 1.505]	0.090 [-0.451, 0.639]	0.667 [0.438, 0.840]	0.886 [0.587, 1.172]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.130, 2.036]	1.239 [0.903, 1.610]	-0.316 [-0.870, 0.215]	0.803 [0.673, 0.904]	1.140 [0.979, 1.341]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.206, 2.133]	1.304 [0.950, 1.705]	-1.061 [-1.545, -0.610]	0.837 [0.729, 0.915]	1.073 [0.932, 1.247]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.058, 2.399]	1.219 [0.844, 1.687]	0.422 [-0.150, 1.044]	0.792 [0.683, 0.898]	1.192 [0.972, 1.483]
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 [1.090, 2.406]	1.250 [0.887, 1.718]	0.467 [-0.093, 1.103]	0.794 [0.688, 0.898]	1.200 [0.980, 1.498]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.370, 2.100]	1.436 [1.095, 1.799]	1.227 [0.780, 1.677]	0.922 [0.862, 0.962]	1.299 [1.124, 1.464]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.591, 2.148]	1.674 [1.361, 1.982]	-0.688 [-1.304, -0.028]	0.531 [0.332, 0.724]	0.670 [0.433, 0.977]
5byn6	Adiabatic scheme for type III submission	1.891 [1.481, 2.268]	1.553 [1.172, 1.948]	1.273 [0.780, 1.782]	0.912 [0.840, 0.959]	1.346 [1.161, 1.524]
y75vj	Direct scheme for type III submission	1.901 [1.505, 2.264]	1.584 [1.225, 1.973]	1.039 [0.469, 1.602]	0.891 [0.789, 0.951]	1.345 [1.161, 1.527]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.213, 2.748]	1.435 [1.040, 1.958]	-0.467 [-1.077, 0.270]	0.709 [0.602, 0.868]	1.083 [0.809, 1.448]
w4iyd	Vertical scheme for type III submission	1.939 [1.537, 2.303]	1.578 [1.185, 1.983]	1.211 [0.665, 1.746]	0.849 [0.717, 0.929]	1.256 [1.020, 1.455]
pwn3m	Analog_search	1.970 [0.784, 2.850]	1.115 [0.567, 1.797]	0.285 [-0.367, 1.090]	0.354 [0.015, 0.894]	0.583 [0.082, 1.034]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.381, 2.953]	1.578 [1.102, 2.156]	-0.733 [-1.428, 0.036]	0.769 [0.668, 0.891]	1.291 [1.012, 1.630]
xikp8	Direct scheme with single point correction for...	2.340 [1.899, 2.720]	2.026 [1.596, 2.449]	0.933 [0.125, 1.702]	0.867 [0.764, 0.932]	1.524 [1.294, 1.787]
5nm4j	Substructure matches from experimental data	2.450 [1.406, 3.324]	1.583 [0.929, 2.334]	0.046 [-0.819, 1.018]	0.192 [0.002, 0.705]	0.398 [-0.065, 0.833]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.592, 3.285]	1.744 [1.139, 2.422]	-0.526 [-1.373, 0.377]	0.726 [0.594, 0.847]	1.373 [1.037, 1.767]
0hxtm	COSMOtherm_FINE17	2.638 [0.879, 3.792]	1.423 [0.664, 2.349]	0.736 [-0.132, 1.783]	0.127 [0.000, 0.837]	0.406 [-0.213, 1.046]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.446, 4.615]	1.883 [1.232, 2.845]	-0.230 [-1.412, 0.700]	0.540 [0.244, 0.882]	1.171 [0.967, 1.383]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.290, 4.738]	1.695 [1.014, 2.744]	-0.773 [-1.965, 0.107]	0.516 [0.219, 0.882]	1.147 [0.951, 1.355]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.462, 4.643]	1.841 [1.182, 2.815]	-0.491 [-1.671, 0.402]	0.547 [0.255, 0.873]	1.192 [0.987, 1.419]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.465, 5.065]	1.985 [1.220, 3.072]	-0.102 [-1.400, 0.942]	0.523 [0.231, 0.873]	1.296 [1.037, 1.604]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.485, 5.058]	1.997 [1.249, 3.079]	-0.138 [-1.418, 0.923]	0.526 [0.237, 0.874]	1.305 [1.046, 1.604]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.890, 6.422]	2.443 [1.514, 3.846]	-0.470 [-2.090, 0.822]	0.486 [0.194, 0.877]	1.435 [1.131, 1.775]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.433, 6.849]	2.999 [1.995, 4.385]	-0.370 [-2.147, 1.102]	0.517 [0.228, 0.880]	1.642 [1.318, 1.985]

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.