ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.546, 0.813]	0.579 [0.451, 0.713]	-0.235 [-0.455, 0.008]	0.937 [0.876, 0.972]	1.015 [0.914, 1.114]
gyuhx	S+pKa	0.730 [0.549, 0.913]	0.579 [0.428, 0.744]	-0.009 [-0.262, 0.261]	0.925 [0.867, 0.963]	0.929 [0.811, 1.028]
xmyhm	ACD/pKa Classic	0.774 [0.495, 1.035]	0.546 [0.365, 0.761]	-0.102 [-0.376, 0.177]	0.916 [0.829, 0.969]	0.934 [0.818, 1.044]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.689, 1.117]	0.710 [0.523, 0.916]	0.288 [-0.028, 0.587]	0.901 [0.817, 0.952]	0.901 [0.772, 1.039]
nb007	Epik-sequential	0.968 [0.768, 1.173]	0.810 [0.632, 1.003]	-0.025 [-0.355, 0.324]	0.871 [0.761, 0.934]	0.997 [0.855, 1.119]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.778, 1.358]	0.814 [0.578, 1.072]	0.475 [0.147, 0.818]	0.906 [0.845, 0.951]	0.840 [0.746, 0.957]
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 [0.522, 1.000]	0.768 [0.558, 1.516]
37xm8	ACD/pKa GALAS	1.358 [0.848, 1.819]	0.955 [0.639, 1.338]	0.101 [-0.391, 0.591]	0.854 [0.726, 0.939]	0.729 [0.599, 0.874]
hytjn	OE Gaussian Process	1.434 [0.990, 1.825]	1.034 [0.690, 1.421]	-0.240 [-0.784, 0.279]	0.675 [0.426, 0.852]	0.795 [0.598, 1.006]
q3pfp	OE Gaussian Process Resampled	1.484 [1.058, 1.871]	1.140 [0.805, 1.506]	-0.090 [-0.655, 0.440]	0.667 [0.433, 0.835]	0.752 [0.568, 0.965]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.137, 2.046]	1.239 [0.908, 1.614]	0.316 [-0.231, 0.882]	0.803 [0.674, 0.903]	0.705 [0.569, 0.837]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.206, 2.142]	1.304 [0.947, 1.713]	1.061 [0.615, 1.544]	0.837 [0.729, 0.917]	0.780 [0.639, 0.926]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.053, 2.389]	1.219 [0.832, 1.685]	-0.422 [-1.031, 0.139]	0.792 [0.682, 0.900]	0.664 [0.519, 0.859]
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 [0.463, 1.000]	0.635 [0.394, 0.785]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.076, 2.406]	1.250 [0.873, 1.705]	-0.467 [-1.080, 0.102]	0.794 [0.687, 0.902]	0.662 [0.517, 0.852]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.362, 2.114]	1.436 [1.083, 1.808]	-1.227 [-1.675, -0.767]	0.922 [0.862, 0.963]	0.710 [0.642, 0.798]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.593, 2.156]	1.674 [1.368, 1.987]	0.688 [0.026, 1.280]	0.531 [0.330, 0.723]	0.793 [0.575, 1.077]
5byn6	Adiabatic scheme for type III submission	1.891 [1.488, 2.274]	1.553 [1.182, 1.946]	-1.273 [-1.774, -0.768]	0.912 [0.843, 0.959]	0.677 [0.613, 0.760]
y75vj	Direct scheme for type III submission	1.901 [1.499, 2.267]	1.584 [1.215, 1.968]	-1.039 [-1.606, -0.462]	0.891 [0.791, 0.951]	0.663 [0.598, 0.735]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.211, 2.698]	1.435 [1.034, 1.945]	0.467 [-0.234, 1.083]	0.709 [0.602, 0.870]	0.655 [0.470, 0.976]
w4iyd	Vertical scheme for type III submission	1.939 [1.530, 2.315]	1.578 [1.185, 1.999]	-1.211 [-1.754, -0.665]	0.849 [0.715, 0.928]	0.676 [0.599, 0.775]
pwn3m	Analog_search	1.970 [0.768, 2.853]	1.115 [0.564, 1.807]	-0.285 [-1.102, 0.396]	0.354 [0.014, 0.895]	0.607 [0.103, 0.874]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.362, 2.956]	1.578 [1.095, 2.173]	0.733 [-0.024, 1.417]	0.769 [0.664, 0.892]	0.596 [0.454, 0.815]
xikp8	Direct scheme with single point correction for...	2.340 [1.912, 2.729]	2.026 [1.603, 2.459]	-0.933 [-1.698, -0.106]	0.867 [0.764, 0.932]	0.569 [0.492, 0.652]
5nm4j	Substructure matches from experimental data	2.450 [1.437, 3.355]	1.583 [0.949, 2.343]	-0.046 [-1.031, 0.783]	0.192 [0.002, 0.696]	0.484 [-0.089, 0.968]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.614, 3.295]	1.744 [1.155, 2.429]	0.526 [-0.371, 1.399]	0.726 [0.593, 0.852]	0.528 [0.407, 0.721]
0hxtm	COSMOtherm_FINE17	2.638 [0.878, 3.813]	1.423 [0.668, 2.351]	-0.736 [-1.800, 0.150]	0.127 [0.000, 0.834]	0.313 [-0.194, 0.777]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.440, 4.619]	1.883 [1.232, 2.832]	0.230 [-0.695, 1.414]	0.540 [0.243, 0.884]	0.461 [0.227, 0.751]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.286, 4.719]	1.695 [1.006, 2.722]	0.773 [-0.111, 1.932]	0.516 [0.218, 0.883]	0.450 [0.207, 0.773]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.459, 4.631]	1.841 [1.182, 2.803]	0.491 [-0.411, 1.639]	0.547 [0.247, 0.874]	0.459 [0.228, 0.739]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.498, 5.043]	1.985 [1.239, 3.059]	0.102 [-0.942, 1.407]	0.523 [0.230, 0.869]	0.404 [0.197, 0.699]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.501, 5.069]	1.997 [1.247, 3.087]	0.138 [-0.906, 1.434]	0.526 [0.232, 0.873]	0.403 [0.195, 0.697]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.893, 6.410]	2.443 [1.511, 3.800]	0.470 [-0.807, 2.095]	0.486 [0.197, 0.878]	0.339 [0.151, 0.629]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.455, 6.879]	2.999 [2.007, 4.413]	0.370 [-1.105, 2.183]	0.517 [0.222, 0.878]	0.315 [0.145, 0.541]

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.