ID	name	RMSE	MAE	ME	R^2	m
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.784, 1.359]	0.814 [0.582, 1.068]	0.475 [0.146, 0.814]	0.906 [0.842, 0.951]	0.840 [0.746, 0.954]
nb007	Epik-sequential	1.208 [0.857, 1.586]	0.935 [0.693, 1.219]	-0.025 [-0.426, 0.415]	0.800 [0.611, 0.915]	0.955 [0.791, 1.088]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.136, 2.045]	1.239 [0.907, 1.621]	0.316 [-0.224, 0.879]	0.803 [0.665, 0.903]	0.705 [0.567, 0.836]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.686 [1.205, 2.137]	1.324 [0.974, 1.718]	0.900 [0.394, 1.421]	0.805 [0.660, 0.904]	0.747 [0.606, 0.893]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.972 [1.278, 2.714]	1.521 [1.149, 1.992]	0.467 [-0.234, 1.085]	0.697 [0.592, 0.858]	0.649 [0.472, 0.962]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.209 [1.424, 2.957]	1.647 [1.179, 2.206]	0.733 [-0.043, 1.435]	0.760 [0.653, 0.886]	0.592 [0.454, 0.804]
yqkga	ReSCoSS conformations // COSMOtherm pKa	2.324 [1.421, 3.098]	1.538 [0.961, 2.219]	-0.123 [-1.021, 0.660]	0.397 [0.085, 0.766]	0.632 [0.299, 0.949]
xmyhm	ACD/pKa Classic	2.333 [1.376, 3.177]	1.486 [0.879, 2.183]	-0.288 [-1.115, 0.586]	0.384 [0.063, 0.770]	0.643 [0.269, 0.887]
pwn3m	Analog_search	3.000 [1.680, 4.077]	1.796 [0.966, 2.759]	-0.904 [-2.042, 0.085]	0.101 [0.000, 0.516]	0.421 [-0.238, 0.822]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.462, 4.636]	1.841 [1.184, 2.811]	0.491 [-0.425, 1.630]	0.547 [0.250, 0.873]	0.459 [0.232, 0.738]
xvxzd	Full quantum chemical calculation of free ener...	3.094 [2.085, 4.026]	2.168 [1.414, 3.013]	-0.427 [-1.537, 0.680]	0.084 [0.000, 0.445]	0.323 [-0.204, 0.757]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	3.096 [1.633, 4.692]	2.044 [1.386, 2.996]	0.069 [-0.911, 1.321]	0.500 [0.204, 0.853]	0.433 [0.204, 0.712]
5nm4j	Substructure matches from experimental data	3.174 [2.363, 3.911]	2.522 [1.819, 3.257]	-0.630 [-1.799, 0.500]	0.040 [0.000, 0.293]	0.247 [-0.330, 0.612]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	3.209 [1.945, 4.311]	2.156 [1.379, 3.083]	-0.602 [-1.783, 0.507]	0.245 [0.022, 0.613]	0.389 [0.108, 0.732]
yc70m	PCM/B3LYP/6-311+G(d,p)	3.298 [2.289, 4.259]	2.493 [1.766, 3.332]	0.218 [-1.010, 1.374]	0.017 [0.000, 0.356]	0.155 [-0.398, 0.780]
gyuhx	S+pKa	3.450 [2.409, 4.361]	2.494 [1.647, 3.402]	-0.430 [-1.673, 0.820]	0.032 [0.000, 0.307]	0.183 [-0.198, 0.582]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	3.581 [1.979, 5.219]	2.368 [1.513, 3.439]	0.361 [-0.858, 1.729]	0.277 [0.050, 0.696]	0.343 [0.116, 0.687]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	3.606 [2.331, 4.778]	2.576 [1.730, 3.562]	0.402 [-0.963, 1.676]	0.309 [0.054, 0.659]	0.350 [0.139, 0.600]
q3pfp	OE Gaussian Process Resampled	3.612 [2.588, 4.543]	2.770 [1.956, 3.642]	-0.772 [-2.070, 0.530]	0.006 [0.000, 0.255]	0.086 [-0.488, 0.502]
p0jba	macroscopic pKa prediction from microscopic pK...	3.667 [2.231, 4.846]	3.276 [1.814, 4.644]	0.320 [-2.844, 3.484]	0.062 [0.002, 1.000]	-0.157 [-2.956, 0.461]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	3.844 [2.922, 4.702]	3.033 [2.221, 3.903]	-0.755 [-2.061, 0.656]	0.072 [0.000, 0.342]	0.205 [-0.099, 0.488]
37xm8	ACD/pKa GALAS	3.967 [2.804, 5.010]	2.792 [1.808, 3.858]	-0.150 [-1.627, 1.270]	0.023 [0.000, 0.346]	0.122 [-0.313, 0.461]
hytjn	OE Gaussian Process	4.037 [2.789, 5.184]	2.980 [2.020, 4.029]	-0.829 [-2.340, 0.621]	0.031 [0.000, 0.286]	-0.201 [-0.628, 0.328]
0hxtm	COSMOtherm_FINE17	4.186 [2.903, 5.382]	3.149 [2.146, 4.286]	-1.643 [-3.144, -0.180]	0.021 [0.000, 0.319]	-0.168 [-0.676, 0.353]
35bdm	macroscopic pKa prediction from microscopic pK...	4.346 [2.777, 5.576]	4.014 [2.520, 5.378]	0.402 [-3.348, 4.152]	0.119 [0.000, 1.000]	-0.179 [-1.215, 0.296]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	4.423 [2.543, 6.098]	2.925 [1.839, 4.242]	-0.051 [-1.626, 1.609]	0.132 [0.002, 0.516]	0.213 [0.012, 0.561]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	4.430 [2.540, 6.130]	2.936 [1.852, 4.277]	-0.014 [-1.592, 1.596]	0.135 [0.003, 0.531]	0.214 [0.017, 0.560]
ryzue	Adiabatic scheme with single point correction ...	4.747 [3.456, 5.938]	3.719 [2.704, 4.840]	-1.507 [-3.083, 0.112]	0.003 [0.000, 0.221]	-0.043 [-0.337, 0.325]
w4iyd	Vertical scheme for type III submission	4.904 [3.576, 6.155]	3.809 [2.752, 4.969]	-1.492 [-3.097, 0.221]	0.017 [0.000, 0.247]	-0.098 [-0.378, 0.265]
5byn6	Adiabatic scheme for type III submission	4.906 [3.629, 6.109]	3.855 [2.820, 4.972]	-1.554 [-3.200, 0.136]	0.005 [0.000, 0.218]	-0.053 [-0.334, 0.289]
y75vj	Direct scheme for type III submission	5.114 [3.625, 6.439]	3.810 [2.650, 5.082]	-1.129 [-2.886, 0.645]	0.016 [0.000, 0.280]	-0.088 [-0.366, 0.243]
xikp8	Direct scheme with single point correction for...	5.193 [3.596, 6.627]	3.859 [2.708, 5.193]	-1.169 [-3.012, 0.662]	0.003 [0.000, 0.275]	0.031 [-0.232, 0.311]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	5.197 [2.909, 7.459]	3.377 [2.099, 4.976]	0.414 [-1.421, 2.421]	0.119 [0.002, 0.519]	0.171 [0.008, 0.476]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	5.635 [3.326, 7.893]	3.884 [2.548, 5.503]	0.324 [-1.670, 2.460]	0.142 [0.003, 0.555]	0.168 [0.012, 0.426]

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.