ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.553, 0.818]	0.579 [0.455, 0.713]	0.235 [-0.000, 0.470]	0.937 [0.875, 0.973]	0.923 [0.838, 1.021]
gyuhx	S+pKa	0.730 [0.547, 0.924]	0.579 [0.418, 0.749]	0.009 [-0.267, 0.283]	0.925 [0.864, 0.964]	0.996 [0.906, 1.117]
xmyhm	ACD/pKa Classic	0.774 [0.499, 1.023]	0.546 [0.369, 0.751]	0.102 [-0.184, 0.349]	0.916 [0.818, 0.968]	0.981 [0.871, 1.112]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.675, 1.125]	0.710 [0.512, 0.908]	-0.288 [-0.571, 0.033]	0.901 [0.821, 0.955]	1.000 [0.855, 1.140]
nb007	Epik-sequential	0.968 [0.755, 1.199]	0.810 [0.622, 1.023]	0.025 [-0.334, 0.353]	0.871 [0.748, 0.933]	0.874 [0.790, 0.979]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.765, 1.362]	0.814 [0.575, 1.073]	-0.475 [-0.805, -0.125]	0.906 [0.844, 0.951]	1.078 [0.938, 1.217]
nb015	Chemicalize v18.23	1.272 [0.992, 1.598]	1.044 [0.803, 1.345]	0.129 [-0.329, 0.578]	0.874 [0.799, 0.934]	1.162 [0.924, 1.371]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.708, 1.728]	1.084 [0.448, 1.720]	-0.924 [-1.720, -0.108]	0.910 [0.509, 1.000]	1.185 [0.339, 1.717]
37xm8	ACD/pKa GALAS	1.358 [0.816, 1.836]	0.955 [0.623, 1.342]	-0.101 [-0.580, 0.449]	0.854 [0.737, 0.940]	1.171 [1.009, 1.378]
hytjn	OE Gaussian Process	1.434 [0.978, 1.818]	1.034 [0.680, 1.411]	0.240 [-0.309, 0.794]	0.675 [0.433, 0.858]	0.849 [0.566, 1.087]
q3pfp	OE Gaussian Process Resampled	1.484 [1.041, 1.850]	1.140 [0.789, 1.496]	0.090 [-0.485, 0.607]	0.667 [0.431, 0.844]	0.886 [0.596, 1.164]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.111, 2.071]	1.239 [0.896, 1.618]	-0.316 [-0.896, 0.241]	0.803 [0.668, 0.907]	1.140 [0.964, 1.333]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.190, 2.157]	1.304 [0.946, 1.729]	-1.061 [-1.510, -0.578]	0.837 [0.728, 0.918]	1.073 [0.929, 1.267]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.050, 2.427]	1.219 [0.846, 1.702]	0.422 [-0.106, 1.015]	0.792 [0.691, 0.895]	1.192 [0.961, 1.479]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.666, 2.372]	1.442 [0.624, 2.262]	-1.006 [-2.178, 0.134]	0.919 [0.463, 1.000]	1.446 [0.735, 2.305]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.074, 2.421]	1.250 [0.872, 1.737]	0.467 [-0.054, 1.134]	0.794 [0.690, 0.903]	1.200 [0.979, 1.492]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.364, 2.098]	1.436 [1.109, 1.780]	1.227 [0.786, 1.657]	0.922 [0.857, 0.964]	1.299 [1.125, 1.475]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.594, 2.145]	1.674 [1.382, 1.986]	-0.688 [-1.292, -0.094]	0.531 [0.330, 0.723]	0.670 [0.443, 0.989]
5byn6	Adiabatic scheme for type III submission	1.891 [1.503, 2.246]	1.553 [1.186, 1.920]	1.273 [0.783, 1.770]	0.912 [0.840, 0.959]	1.346 [1.158, 1.522]
y75vj	Direct scheme for type III submission	1.901 [1.521, 2.257]	1.584 [1.216, 1.971]	1.039 [0.489, 1.632]	0.891 [0.785, 0.954]	1.345 [1.164, 1.543]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.214, 2.747]	1.435 [1.031, 1.956]	-0.467 [-1.096, 0.231]	0.709 [0.603, 0.870]	1.083 [0.809, 1.456]
w4iyd	Vertical scheme for type III submission	1.939 [1.528, 2.311]	1.578 [1.161, 1.989]	1.211 [0.665, 1.757]	0.849 [0.704, 0.926]	1.256 [0.991, 1.452]
pwn3m	Analog_search	1.970 [0.796, 2.917]	1.115 [0.568, 1.863]	0.285 [-0.397, 1.173]	0.354 [0.022, 0.902]	0.583 [0.113, 1.032]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.342, 2.928]	1.578 [1.078, 2.133]	-0.733 [-1.387, 0.015]	0.769 [0.678, 0.893]	1.291 [1.021, 1.607]
xikp8	Direct scheme with single point correction for...	2.340 [1.900, 2.732]	2.026 [1.601, 2.452]	0.933 [0.094, 1.705]	0.867 [0.751, 0.935]	1.524 [1.277, 1.763]
5nm4j	Substructure matches from experimental data	2.450 [1.420, 3.407]	1.583 [0.946, 2.396]	0.046 [-0.832, 1.102]	0.192 [0.002, 0.725]	0.398 [-0.089, 0.862]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.607, 3.246]	1.744 [1.160, 2.390]	-0.526 [-1.347, 0.350]	0.726 [0.614, 0.848]	1.373 [1.043, 1.808]
0hxtm	COSMOtherm_FINE17	2.638 [0.870, 3.734]	1.423 [0.668, 2.272]	0.736 [-0.118, 1.701]	0.127 [0.000, 0.827]	0.406 [-0.238, 1.044]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.455, 5.012]	1.883 [1.235, 2.953]	-0.230 [-1.631, 0.741]	0.540 [0.225, 0.886]	1.171 [0.946, 1.374]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.289, 4.761]	1.695 [1.027, 2.806]	-0.773 [-1.935, 0.136]	0.516 [0.231, 0.878]	1.147 [0.969, 1.357]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.464, 4.642]	1.841 [1.179, 2.829]	-0.491 [-1.657, 0.483]	0.547 [0.247, 0.877]	1.192 [0.976, 1.426]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.537, 4.998]	1.985 [1.241, 2.989]	-0.102 [-1.332, 1.019]	0.523 [0.227, 0.872]	1.296 [1.034, 1.580]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.506, 5.072]	1.997 [1.256, 3.035]	-0.138 [-1.368, 0.917]	0.526 [0.234, 0.874]	1.305 [1.046, 1.606]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.905, 6.415]	2.443 [1.505, 3.766]	-0.470 [-2.108, 0.899]	0.486 [0.205, 0.877]	1.435 [1.132, 1.800]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.430, 6.905]	2.999 [1.978, 4.372]	-0.370 [-2.099, 0.930]	0.517 [0.214, 0.886]	1.642 [1.302, 2.019]

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.