ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.540, 0.818]	0.579 [0.451, 0.712]	0.235 [-0.002, 0.466]	0.937 [0.881, 0.973]	0.923 [0.843, 1.019]
gyuhx	S+pKa	0.732 [0.547, 0.908]	0.585 [0.431, 0.754]	0.035 [-0.226, 0.280]	0.929 [0.880, 0.967]	0.979 [0.903, 1.080]
xmyhm	ACD/pKa Classic	0.787 [0.517, 1.041]	0.564 [0.376, 0.778]	0.134 [-0.149, 0.400]	0.919 [0.844, 0.967]	0.961 [0.852, 1.081]
nb007	Epik-sequential	0.968 [0.761, 1.170]	0.810 [0.628, 1.004]	0.025 [-0.341, 0.368]	0.871 [0.755, 0.938]	0.874 [0.783, 0.987]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.787, 1.240]	0.799 [0.604, 1.020]	-0.166 [-0.513, 0.206]	0.867 [0.785, 0.933]	0.927 [0.763, 1.084]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.770, 1.367]	0.814 [0.569, 1.102]	-0.475 [-0.869, -0.149]	0.906 [0.845, 0.954]	1.078 [0.939, 1.217]
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 [0.428, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.933, 1.899]	1.008 [0.682, 1.425]	-0.183 [-0.675, 0.342]	0.834 [0.698, 0.929]	1.155 [0.979, 1.343]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.165, 2.035]	1.239 [0.923, 1.625]	-0.316 [-0.840, 0.241]	0.803 [0.673, 0.904]	1.140 [0.974, 1.351]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.217, 2.104]	1.296 [0.969, 1.692]	-0.122 [-0.719, 0.462]	0.813 [0.683, 0.904]	1.198 [1.041, 1.401]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.043, 2.366]	1.213 [0.837, 1.674]	0.442 [-0.136, 1.005]	0.797 [0.708, 0.903]	1.156 [0.962, 1.420]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.091, 2.438]	1.246 [0.888, 1.708]	0.509 [-0.033, 1.119]	0.796 [0.709, 0.893]	1.153 [0.939, 1.433]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	-1.006 [-2.178, 0.136]	0.919 [0.457, 1.000]	1.446 [0.735, 2.305]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.435, 2.142]	1.500 [1.182, 1.873]	1.298 [0.883, 1.704]	0.910 [0.862, 0.949]	1.229 [1.061, 1.428]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.277, 2.283]	1.389 [0.995, 1.838]	-0.744 [-1.329, -0.153]	0.792 [0.667, 0.893]	1.149 [0.960, 1.384]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.369, 2.239]	1.482 [1.108, 1.883]	0.103 [-0.580, 0.747]	0.820 [0.699, 0.908]	1.294 [1.108, 1.509]
5byn6	Adiabatic scheme for type III submission	1.890 [1.482, 2.242]	1.588 [1.229, 1.942]	1.317 [0.821, 1.767]	0.905 [0.854, 0.948]	1.284 [1.098, 1.465]
y75vj	Direct scheme for type III submission	1.901 [1.494, 2.265]	1.584 [1.217, 1.978]	1.039 [0.457, 1.651]	0.891 [0.792, 0.949]	1.345 [1.159, 1.535]
w4iyd	Vertical scheme for type III submission	1.926 [1.524, 2.298]	1.584 [1.207, 2.012]	1.257 [0.757, 1.761]	0.853 [0.744, 0.923]	1.206 [1.000, 1.419]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.189, 2.684]	1.435 [1.011, 1.919]	-0.467 [-1.093, 0.251]	0.709 [0.603, 0.879]	1.083 [0.799, 1.442]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.367, 2.621]	1.568 [1.169, 2.021]	0.557 [-0.130, 1.187]	0.823 [0.715, 0.908]	1.350 [1.145, 1.596]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.418, 2.675]	1.577 [1.193, 2.084]	0.524 [-0.095, 1.233]	0.825 [0.728, 0.907]	1.358 [1.160, 1.626]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.664, 2.316]	1.805 [1.442, 2.120]	-0.405 [-1.125, 0.370]	0.469 [0.295, 0.656]	0.559 [0.355, 0.865]
hytjn	OE Gaussian Process	2.161 [1.251, 3.070]	1.389 [0.861, 2.044]	0.709 [0.015, 1.482]	0.449 [0.131, 0.788]	0.621 [0.270, 1.018]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.408, 3.022]	1.578 [1.119, 2.205]	-0.733 [-1.409, 0.083]	0.769 [0.673, 0.888]	1.291 [1.018, 1.642]
q3pfp	OE Gaussian Process Resampled	2.193 [1.294, 3.022]	1.505 [0.965, 2.120]	0.589 [-0.088, 1.380]	0.443 [0.126, 0.783]	0.658 [0.257, 1.082]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.620, 2.755]	1.778 [1.319, 2.235]	0.784 [0.130, 1.484]	0.822 [0.697, 0.913]	1.406 [1.203, 1.621]
xikp8	Direct scheme with single point correction for...	2.348 [1.925, 2.713]	2.056 [1.634, 2.455]	0.773 [-0.026, 1.548]	0.890 [0.784, 0.947]	1.588 [1.385, 1.799]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.781, 2.917]	1.915 [1.432, 2.385]	0.313 [-0.484, 1.223]	0.842 [0.749, 0.915]	1.557 [1.333, 1.813]
5nm4j	Substructure matches from experimental data	2.450 [1.389, 3.504]	1.583 [0.907, 2.491]	0.046 [-0.802, 1.188]	0.192 [0.002, 0.726]	0.398 [-0.137, 0.810]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.643, 3.259]	1.826 [1.243, 2.460]	-0.651 [-1.473, 0.229]	0.761 [0.633, 0.879]	1.432 [1.119, 1.747]
pwn3m	Analog_search	2.604 [1.356, 3.577]	1.539 [0.786, 2.450]	0.788 [-0.076, 1.860]	0.208 [0.003, 0.671]	0.369 [0.001, 0.820]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.382, 3.597]	2.525 [1.989, 3.124]	0.424 [-0.629, 1.499]	0.844 [0.746, 0.915]	1.784 [1.548, 2.067]
0hxtm	COSMOtherm_FINE17	3.263 [1.719, 4.402]	1.918 [0.991, 2.999]	1.377 [0.318, 2.538]	0.075 [0.000, 0.547]	0.281 [-0.157, 0.905]

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.