ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.546, 0.812]	0.579 [0.451, 0.712]	0.235 [-0.002, 0.461]	0.937 [0.878, 0.972]	0.923 [0.837, 1.016]
gyuhx	S+pKa	0.730 [0.546, 0.913]	0.579 [0.427, 0.749]	0.009 [-0.254, 0.263]	0.925 [0.867, 0.964]	0.996 [0.910, 1.109]
xmyhm	ACD/pKa Classic	0.774 [0.493, 1.030]	0.546 [0.360, 0.759]	0.102 [-0.180, 0.374]	0.916 [0.831, 0.970]	0.981 [0.869, 1.106]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.681, 1.117]	0.710 [0.517, 0.915]	-0.288 [-0.582, 0.023]	0.901 [0.821, 0.953]	1.000 [0.868, 1.123]
nb007	nb007-976-typeIII-epik_scan-1	0.946 [0.731, 1.160]	0.776 [0.594, 0.973]	0.045 [-0.297, 0.370]	0.879 [0.760, 0.944]	0.840 [0.769, 0.922]
nb010	nb010-976-typeIII-epik_microscopic-1	1.028 [0.769, 1.269]	0.814 [0.605, 1.045]	0.243 [-0.123, 0.594]	0.869 [0.769, 0.940]	0.946 [0.823, 1.077]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.781, 1.362]	0.814 [0.576, 1.073]	-0.475 [-0.823, -0.143]	0.906 [0.841, 0.951]	1.078 [0.936, 1.217]
nb013	nb013-976-typeIII-jaguar-1	1.103 [0.710, 1.475]	0.803 [0.558, 1.090]	-0.148 [-0.555, 0.219]	0.884 [0.784, 0.946]	1.092 [0.904, 1.254]
nb015	Chemicalize v18.23	1.272 [0.980, 1.569]	1.044 [0.796, 1.308]	0.129 [-0.330, 0.549]	0.874 [0.798, 0.933]	1.162 [0.942, 1.337]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.718]	1.084 [0.428, 1.704]	-0.924 [-1.704, -0.108]	0.910 [0.509, 1.000]	1.185 [0.339, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.846, 1.816]	0.955 [0.640, 1.328]	-0.101 [-0.594, 0.388]	0.854 [0.731, 0.939]	1.171 [0.996, 1.350]
hytjn	OE Gaussian Process	1.434 [0.985, 1.828]	1.034 [0.687, 1.422]	0.240 [-0.280, 0.767]	0.675 [0.422, 0.851]	0.849 [0.558, 1.100]
q3pfp	OE Gaussian Process Resampled	1.484 [1.061, 1.867]	1.140 [0.809, 1.504]	0.090 [-0.443, 0.641]	0.667 [0.430, 0.838]	0.886 [0.587, 1.178]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.137, 2.042]	1.239 [0.903, 1.615]	-0.316 [-0.879, 0.215]	0.803 [0.672, 0.903]	1.140 [0.978, 1.338]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.200, 2.125]	1.304 [0.952, 1.694]	-1.061 [-1.528, -0.616]	0.837 [0.729, 0.916]	1.073 [0.932, 1.250]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.057, 2.400]	1.219 [0.844, 1.688]	0.422 [-0.137, 1.027]	0.792 [0.688, 0.899]	1.192 [0.970, 1.482]
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 [0.720, 2.147]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.083, 2.398]	1.250 [0.883, 1.721]	0.467 [-0.095, 1.086]	0.794 [0.684, 0.901]	1.200 [0.977, 1.493]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.361, 2.106]	1.436 [1.085, 1.793]	1.227 [0.783, 1.672]	0.922 [0.860, 0.963]	1.299 [1.127, 1.468]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.583, 2.153]	1.674 [1.356, 1.987]	-0.688 [-1.290, -0.023]	0.531 [0.331, 0.726]	0.670 [0.426, 0.979]
5byn6	Adiabatic scheme for type III submission	1.891 [1.480, 2.278]	1.553 [1.170, 1.953]	1.273 [0.768, 1.786]	0.912 [0.841, 0.959]	1.346 [1.160, 1.528]
y75vj	Direct scheme for type III submission	1.901 [1.503, 2.266]	1.584 [1.216, 1.975]	1.039 [0.463, 1.628]	0.891 [0.790, 0.951]	1.345 [1.159, 1.531]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.208, 2.702]	1.435 [1.034, 1.936]	-0.467 [-1.073, 0.246]	0.709 [0.604, 0.868]	1.083 [0.808, 1.443]
w4iyd	Vertical scheme for type III submission	1.939 [1.533, 2.304]	1.578 [1.184, 1.987]	1.211 [0.657, 1.743]	0.849 [0.713, 0.928]	1.256 [1.007, 1.457]
pwn3m	Analog_search	1.970 [0.787, 2.841]	1.115 [0.567, 1.802]	0.285 [-0.366, 1.105]	0.354 [0.014, 0.895]	0.583 [0.070, 1.033]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.375, 2.958]	1.578 [1.092, 2.166]	-0.733 [-1.422, 0.035]	0.769 [0.666, 0.892]	1.291 [1.010, 1.640]
xikp8	Direct scheme with single point correction for...	2.340 [1.908, 2.737]	2.026 [1.604, 2.462]	0.933 [0.129, 1.696]	0.867 [0.766, 0.932]	1.524 [1.294, 1.772]
5nm4j	Substructure matches from experimental data	2.450 [1.399, 3.356]	1.583 [0.933, 2.368]	0.046 [-0.801, 1.041]	0.192 [0.002, 0.692]	0.398 [-0.066, 0.818]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.623, 3.298]	1.744 [1.158, 2.425]	-0.526 [-1.385, 0.369]	0.726 [0.596, 0.847]	1.373 [1.041, 1.776]
0hxtm	COSMOtherm_FINE17	2.638 [0.874, 3.815]	1.423 [0.660, 2.372]	0.736 [-0.143, 1.818]	0.127 [0.000, 0.838]	0.406 [-0.230, 1.055]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.439, 4.641]	1.883 [1.233, 2.885]	-0.230 [-1.464, 0.703]	0.540 [0.239, 0.884]	1.171 [0.962, 1.379]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.279, 4.733]	1.695 [1.010, 2.734]	-0.773 [-1.967, 0.121]	0.516 [0.222, 0.886]	1.147 [0.954, 1.364]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.464, 4.631]	1.841 [1.182, 2.793]	-0.491 [-1.640, 0.415]	0.547 [0.253, 0.875]	1.192 [0.993, 1.416]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.481, 5.057]	1.985 [1.222, 3.053]	-0.102 [-1.428, 0.959]	0.523 [0.233, 0.874]	1.296 [1.040, 1.597]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.514, 5.068]	1.997 [1.252, 3.074]	-0.138 [-1.421, 0.915]	0.526 [0.235, 0.871]	1.305 [1.049, 1.597]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.888, 6.412]	2.443 [1.514, 3.796]	-0.470 [-2.082, 0.837]	0.486 [0.197, 0.878]	1.435 [1.137, 1.772]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.428, 6.863]	2.999 [1.995, 4.406]	-0.370 [-2.112, 1.102]	0.517 [0.224, 0.880]	1.642 [1.322, 1.983]

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.