ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.542, 0.815]	0.579 [0.448, 0.714]	0.235 [0.001, 0.458]	0.937 [0.877, 0.972]	0.923 [0.836, 1.015]
gyuhx	S+pKa	0.730 [0.548, 0.918]	0.579 [0.427, 0.748]	0.009 [-0.266, 0.266]	0.925 [0.868, 0.963]	0.996 [0.912, 1.112]
xmyhm	ACD/pKa Classic	0.774 [0.494, 1.029]	0.546 [0.363, 0.757]	0.102 [-0.166, 0.372]	0.916 [0.830, 0.968]	0.981 [0.869, 1.106]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.684, 1.121]	0.710 [0.517, 0.917]	-0.288 [-0.580, 0.027]	0.901 [0.823, 0.954]	1.000 [0.867, 1.125]
nb007	Epik-sequential	0.968 [0.763, 1.170]	0.810 [0.626, 1.000]	0.025 [-0.323, 0.356]	0.871 [0.762, 0.934]	0.874 [0.787, 0.979]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.779, 1.357]	0.814 [0.574, 1.065]	-0.475 [-0.812, -0.148]	0.906 [0.842, 0.952]	1.078 [0.935, 1.219]
nb015	Chemicalize v18.23	1.272 [0.985, 1.567]	1.044 [0.797, 1.310]	0.129 [-0.331, 0.565]	0.874 [0.796, 0.931]	1.162 [0.935, 1.338]
nb014	Chemicalize v18.12	1.278 [0.976, 1.585]	1.033 [0.775, 1.314]	0.165 [-0.307, 0.614]	0.877 [0.794, 0.936]	1.200 [0.965, 1.384]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.708, 1.728]	1.084 [0.428, 1.720]	-0.924 [-1.720, -0.108]	0.910 [0.522, 1.000]	1.185 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.848, 1.816]	0.955 [0.632, 1.343]	-0.101 [-0.593, 0.390]	0.854 [0.726, 0.938]	1.171 [0.996, 1.355]
hytjn	OE Gaussian Process	1.434 [0.976, 1.825]	1.034 [0.684, 1.411]	0.240 [-0.270, 0.765]	0.675 [0.422, 0.854]	0.849 [0.551, 1.101]
q3pfp	OE Gaussian Process Resampled	1.484 [1.050, 1.868]	1.140 [0.806, 1.504]	0.090 [-0.446, 0.649]	0.667 [0.429, 0.839]	0.886 [0.587, 1.174]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.144, 2.041]	1.239 [0.906, 1.613]	-0.316 [-0.884, 0.224]	0.803 [0.666, 0.904]	1.140 [0.978, 1.341]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.206, 2.139]	1.304 [0.954, 1.699]	-1.061 [-1.543, -0.616]	0.837 [0.731, 0.916]	1.073 [0.935, 1.252]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.054, 2.393]	1.219 [0.839, 1.688]	0.422 [-0.139, 1.049]	0.792 [0.680, 0.899]	1.192 [0.970, 1.490]
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 [1.073, 2.420]	1.250 [0.871, 1.721]	0.467 [-0.096, 1.093]	0.794 [0.688, 0.902]	1.200 [0.974, 1.485]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.364, 2.106]	1.436 [1.088, 1.802]	1.227 [0.775, 1.670]	0.922 [0.861, 0.962]	1.299 [1.131, 1.463]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.589, 2.152]	1.674 [1.361, 1.984]	-0.688 [-1.309, -0.036]	0.531 [0.332, 0.721]	0.670 [0.429, 0.973]
5byn6	Adiabatic scheme for type III submission	1.891 [1.491, 2.267]	1.553 [1.176, 1.942]	1.273 [0.781, 1.764]	0.912 [0.841, 0.958]	1.346 [1.165, 1.527]
y75vj	Direct scheme for type III submission	1.901 [1.499, 2.257]	1.584 [1.212, 1.964]	1.039 [0.478, 1.605]	0.891 [0.789, 0.950]	1.345 [1.157, 1.533]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.222, 2.724]	1.435 [1.044, 1.948]	-0.467 [-1.070, 0.236]	0.709 [0.602, 0.868]	1.083 [0.810, 1.445]
w4iyd	Vertical scheme for type III submission	1.939 [1.520, 2.308]	1.578 [1.178, 1.993]	1.211 [0.668, 1.733]	0.849 [0.715, 0.928]	1.256 [1.018, 1.459]
pwn3m	Analog_search	1.970 [0.776, 2.870]	1.115 [0.572, 1.803]	0.285 [-0.390, 1.102]	0.354 [0.019, 0.903]	0.583 [0.088, 1.039]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.369, 2.953]	1.578 [1.094, 2.148]	-0.733 [-1.429, 0.038]	0.769 [0.670, 0.891]	1.291 [1.013, 1.631]
xikp8	Direct scheme with single point correction for...	2.340 [1.916, 2.734]	2.026 [1.614, 2.462]	0.933 [0.131, 1.678]	0.867 [0.762, 0.932]	1.524 [1.298, 1.785]
5nm4j	Substructure matches from experimental data	2.450 [1.426, 3.319]	1.583 [0.938, 2.318]	0.046 [-0.799, 1.003]	0.192 [0.002, 0.693]	0.398 [-0.057, 0.818]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.602, 3.308]	1.744 [1.141, 2.444]	-0.526 [-1.378, 0.362]	0.726 [0.595, 0.847]	1.373 [1.041, 1.773]
0hxtm	COSMOtherm_FINE17	2.638 [0.862, 3.800]	1.423 [0.655, 2.361]	0.736 [-0.143, 1.808]	0.127 [0.000, 0.839]	0.406 [-0.217, 1.055]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.449, 4.603]	1.883 [1.241, 2.832]	-0.230 [-1.408, 0.695]	0.540 [0.242, 0.881]	1.171 [0.962, 1.375]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.285, 4.695]	1.695 [1.014, 2.691]	-0.773 [-1.899, 0.105]	0.516 [0.227, 0.883]	1.147 [0.963, 1.356]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.442, 4.638]	1.841 [1.162, 2.795]	-0.491 [-1.673, 0.438]	0.547 [0.252, 0.877]	1.192 [0.976, 1.421]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.468, 5.057]	1.985 [1.226, 3.053]	-0.102 [-1.370, 0.966]	0.523 [0.236, 0.872]	1.296 [1.039, 1.594]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.495, 5.085]	1.997 [1.244, 3.083]	-0.138 [-1.459, 0.916]	0.526 [0.236, 0.874]	1.305 [1.045, 1.610]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.873, 6.404]	2.443 [1.501, 3.796]	-0.470 [-2.120, 0.807]	0.486 [0.199, 0.881]	1.435 [1.134, 1.780]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.430, 6.864]	2.999 [1.999, 4.432]	-0.370 [-2.151, 1.093]	0.517 [0.224, 0.882]	1.642 [1.316, 1.989]

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.