ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.546, 0.811]	0.579 [0.452, 0.712]	0.235 [-0.001, 0.464]	0.937 [0.878, 0.973]	0.923 [0.836, 1.016]
gyuhx	S+pKa	0.730 [0.547, 0.911]	0.579 [0.424, 0.745]	0.009 [-0.263, 0.260]	0.925 [0.871, 0.963]	0.996 [0.910, 1.108]
xmyhm	ACD/pKa Classic	0.774 [0.494, 1.034]	0.546 [0.367, 0.758]	0.102 [-0.178, 0.376]	0.916 [0.831, 0.968]	0.981 [0.870, 1.105]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.679, 1.126]	0.710 [0.514, 0.920]	-0.288 [-0.579, 0.038]	0.901 [0.821, 0.954]	1.000 [0.866, 1.127]
nb007	Epik Scan	0.946 [0.726, 1.152]	0.776 [0.587, 0.967]	0.045 [-0.296, 0.369]	0.879 [0.765, 0.945]	0.840 [0.768, 0.923]
nb010	Epik Microscopic	1.028 [0.763, 1.267]	0.814 [0.597, 1.040]	0.243 [-0.114, 0.594]	0.869 [0.771, 0.940]	0.946 [0.828, 1.080]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.785, 1.366]	0.814 [0.581, 1.076]	-0.475 [-0.819, -0.141]	0.906 [0.839, 0.952]	1.078 [0.939, 1.221]
nb013	Jaguar	1.103 [0.716, 1.478]	0.803 [0.561, 1.091]	-0.148 [-0.559, 0.212]	0.884 [0.783, 0.947]	1.092 [0.904, 1.254]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.987, 1.581]	1.044 [0.803, 1.318]	0.129 [-0.335, 0.560]	0.874 [0.795, 0.933]	1.162 [0.944, 1.341]
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 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.358 [0.839, 1.825]	0.955 [0.631, 1.344]	-0.101 [-0.593, 0.407]	0.854 [0.733, 0.939]	1.171 [1.001, 1.355]
hytjn	OE Gaussian Process	1.434 [0.983, 1.826]	1.034 [0.685, 1.420]	0.240 [-0.277, 0.771]	0.675 [0.421, 0.854]	0.849 [0.556, 1.100]
q3pfp	OE Gaussian Process Resampled	1.484 [1.053, 1.863]	1.140 [0.805, 1.505]	0.090 [-0.446, 0.640]	0.667 [0.432, 0.838]	0.886 [0.588, 1.171]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.140, 2.040]	1.239 [0.907, 1.615]	-0.316 [-0.879, 0.229]	0.803 [0.664, 0.903]	1.140 [0.981, 1.344]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.213, 2.141]	1.304 [0.958, 1.708]	-1.061 [-1.537, -0.607]	0.837 [0.727, 0.914]	1.073 [0.933, 1.247]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.053, 2.395]	1.219 [0.838, 1.697]	0.422 [-0.141, 1.051]	0.792 [0.681, 0.900]	1.192 [0.971, 1.484]
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 [0.735, 2.147]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.089, 2.400]	1.250 [0.881, 1.716]	0.467 [-0.103, 1.097]	0.794 [0.684, 0.898]	1.200 [0.971, 1.498]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.371, 2.105]	1.436 [1.092, 1.799]	1.227 [0.786, 1.675]	0.922 [0.862, 0.962]	1.299 [1.126, 1.465]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.595, 2.152]	1.674 [1.368, 1.980]	-0.688 [-1.295, -0.046]	0.531 [0.334, 0.721]	0.670 [0.427, 0.969]
5byn6	Adiabatic scheme for type III submission	1.891 [1.492, 2.281]	1.553 [1.176, 1.956]	1.273 [0.786, 1.780]	0.912 [0.841, 0.959]	1.346 [1.159, 1.529]
y75vj	Direct scheme for type III submission	1.901 [1.503, 2.266]	1.584 [1.217, 1.970]	1.039 [0.463, 1.616]	0.891 [0.790, 0.950]	1.345 [1.162, 1.528]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.214, 2.715]	1.435 [1.037, 1.939]	-0.467 [-1.074, 0.253]	0.709 [0.599, 0.868]	1.083 [0.801, 1.446]
w4iyd	Vertical scheme for type III submission	1.939 [1.521, 2.294]	1.578 [1.180, 1.979]	1.211 [0.667, 1.746]	0.849 [0.710, 0.927]	1.256 [1.015, 1.454]
pwn3m	Analog_search	1.970 [0.785, 2.866]	1.115 [0.572, 1.805]	0.285 [-0.376, 1.117]	0.354 [0.015, 0.897]	0.583 [0.074, 1.030]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.376, 2.966]	1.578 [1.092, 2.160]	-0.733 [-1.404, 0.045]	0.769 [0.667, 0.891]	1.291 [1.009, 1.639]
xikp8	Direct scheme with single point correction for...	2.340 [1.904, 2.723]	2.026 [1.600, 2.447]	0.933 [0.144, 1.716]	0.867 [0.762, 0.932]	1.524 [1.293, 1.778]
5nm4j	Substructure matches from experimental data	2.450 [1.407, 3.332]	1.583 [0.941, 2.336]	0.046 [-0.802, 0.995]	0.192 [0.002, 0.704]	0.398 [-0.068, 0.836]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.606, 3.293]	1.744 [1.149, 2.432]	-0.526 [-1.397, 0.377]	0.726 [0.594, 0.848]	1.373 [1.043, 1.772]
0hxtm	COSMOtherm_FINE17	2.638 [0.875, 3.787]	1.423 [0.677, 2.352]	0.736 [-0.142, 1.798]	0.127 [0.000, 0.835]	0.406 [-0.231, 1.041]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.450, 4.610]	1.883 [1.236, 2.838]	-0.230 [-1.384, 0.676]	0.540 [0.243, 0.880]	1.171 [0.964, 1.376]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.276, 4.711]	1.695 [1.009, 2.693]	-0.773 [-1.909, 0.111]	0.516 [0.225, 0.884]	1.147 [0.956, 1.360]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.482, 4.643]	1.841 [1.192, 2.802]	-0.491 [-1.646, 0.399]	0.547 [0.255, 0.873]	1.192 [0.982, 1.423]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.489, 5.087]	1.985 [1.235, 3.066]	-0.102 [-1.409, 0.946]	0.523 [0.231, 0.868]	1.296 [1.034, 1.596]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.494, 5.083]	1.997 [1.244, 3.070]	-0.138 [-1.408, 0.942]	0.526 [0.233, 0.873]	1.305 [1.042, 1.598]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.894, 6.390]	2.443 [1.522, 3.781]	-0.470 [-2.081, 0.800]	0.486 [0.195, 0.878]	1.435 [1.129, 1.764]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.429, 6.862]	2.999 [1.995, 4.406]	-0.370 [-2.147, 1.137]	0.517 [0.225, 0.881]	1.642 [1.315, 1.987]

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.