ID	name	RMSE	MAE	ME	R^2	m
hdiyq	S+pKa	0.627 [0.461, 0.772]	0.478 [0.327, 0.638]	0.152 [-0.090, 0.382]	0.948 [0.910, 0.976]	1.038 [0.948, 1.162]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.431, 0.848]	0.495 [0.339, 0.675]	0.026 [-0.233, 0.291]	0.936 [0.849, 0.977]	0.978 [0.901, 1.051]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.462, 0.835]	0.520 [0.377, 0.682]	-0.089 [-0.343, 0.166]	0.943 [0.860, 0.980]	1.039 [0.969, 1.091]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.431, 0.905]	0.495 [0.317, 0.688]	0.058 [-0.199, 0.331]	0.924 [0.844, 0.974]	0.961 [0.847, 1.064]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.426, 0.961]	0.480 [0.294, 0.696]	0.159 [-0.098, 0.440]	0.920 [0.827, 0.974]	0.939 [0.834, 1.051]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.618, 0.956]	0.639 [0.461, 0.828]	-0.243 [-0.537, 0.051]	0.911 [0.819, 0.958]	0.981 [0.821, 1.088]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.638, 1.162]	0.698 [0.476, 0.942]	0.276 [-0.060, 0.618]	0.892 [0.772, 0.955]	0.997 [0.876, 1.117]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.932 [0.549, 1.259]	0.655 [0.423, 0.925]	0.118 [-0.228, 0.480]	0.861 [0.670, 0.961]	0.878 [0.764, 0.955]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.664, 1.183]	0.711 [0.486, 0.950]	0.172 [-0.167, 0.528]	0.870 [0.756, 0.939]	0.950 [0.818, 1.123]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.594, 1.348]	0.694 [0.460, 0.971]	-0.003 [-0.384, 0.353]	0.853 [0.657, 0.955]	0.920 [0.801, 1.011]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	1.041 [0.602, 1.434]	0.730 [0.468, 1.037]	0.036 [-0.355, 0.453]	0.871 [0.682, 0.968]	1.075 [0.932, 1.170]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.729, 1.355]	0.766 [0.509, 1.050]	-0.409 [-0.785, -0.058]	0.915 [0.821, 0.963]	1.160 [0.995, 1.296]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.456, 1.671]	0.611 [0.329, 1.009]	0.126 [-0.238, 0.588]	0.892 [0.800, 0.975]	1.144 [0.968, 1.361]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.482, 1.673]	0.629 [0.345, 1.020]	0.085 [-0.295, 0.551]	0.892 [0.802, 0.973]	1.152 [0.971, 1.356]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.516, 1.665]	0.665 [0.392, 1.049]	0.238 [-0.123, 0.690]	0.851 [0.765, 0.956]	1.020 [0.821, 1.294]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.512, 1.678]	0.659 [0.376, 1.043]	0.225 [-0.147, 0.683]	0.858 [0.781, 0.958]	1.050 [0.846, 1.324]
arcko	Vertical scheme for type I submission	1.095 [0.746, 1.410]	0.815 [0.548, 1.112]	0.434 [0.061, 0.827]	0.865 [0.759, 0.933]	1.024 [0.896, 1.202]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.826, 1.354]	0.893 [0.653, 1.149]	0.440 [0.048, 0.825]	0.890 [0.759, 0.957]	1.112 [0.964, 1.255]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.521, 1.688]	0.675 [0.397, 1.061]	0.095 [-0.289, 0.564]	0.872 [0.790, 0.964]	1.118 [0.954, 1.364]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.792, 1.454]	0.863 [0.599, 1.167]	-0.367 [-0.800, 0.038]	0.895 [0.801, 0.949]	1.168 [1.030, 1.343]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.296, 1.647]	0.884 [0.228, 1.540]	-0.764 [-1.540, 0.012]	0.914 [0.457, 1.000]	1.162 [0.519, 1.592]
wcvnu	Adiabatic scheme for type I submission	1.190 [0.871, 1.493]	0.960 [0.702, 1.247]	0.331 [-0.111, 0.770]	0.862 [0.700, 0.943]	1.115 [0.963, 1.277]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.648, 1.813]	0.794 [0.464, 1.212]	0.132 [-0.315, 0.654]	0.861 [0.779, 0.952]	1.152 [0.976, 1.429]
wexjs	Direct scheme for type I submission	1.426 [1.062, 1.767]	1.154 [0.838, 1.495]	0.315 [-0.220, 0.876]	0.828 [0.639, 0.925]	1.187 [0.986, 1.406]
v8qph	ACD/pKa GALAS	1.486 [0.995, 1.910]	1.080 [0.706, 1.490]	-0.164 [-0.738, 0.411]	0.813 [0.610, 0.927]	1.226 [0.970, 1.431]
w4z0e	Direct scheme with single point correction for...	1.699 [1.268, 2.081]	1.390 [1.022, 1.780]	0.175 [-0.492, 0.823]	0.843 [0.727, 0.917]	1.353 [1.132, 1.640]
6tvf8	OE Gaussian Process	2.031 [0.901, 3.098]	1.131 [0.567, 1.870]	0.462 [-0.233, 1.303]	0.324 [0.023, 0.807]	0.432 [0.088, 0.868]
0wfzo	Explicit solvent submission 1	2.968 [1.637, 4.101]	1.957 [1.187, 2.882]	0.642 [-0.400, 1.802]	0.355 [0.084, 0.707]	0.862 [0.367, 1.363]
t8ewk	COSMOlogic_FINE17	3.128 [1.629, 4.348]	1.801 [0.870, 2.935]	1.260 [0.207, 2.525]	0.092 [0.000, 0.569]	0.313 [-0.162, 0.938]
z3btx	Explicit solvent submission 2	3.692 [1.771, 5.346]	2.243 [1.252, 3.497]	1.049 [-0.210, 2.552]	0.178 [0.002, 0.656]	0.643 [-0.063, 1.269]
758j8	Explicit solvent submission 3	4.214 [2.095, 6.092]	2.743 [1.670, 4.076]	1.512 [0.128, 3.155]	0.123 [0.001, 0.582]	0.572 [-0.213, 1.302]
hgn83	Explicit solvent submission 4	6.196 [3.431, 8.571]	3.985 [2.309, 5.987]	2.711 [0.677, 4.955]	0.022 [0.000, 0.332]	0.321 [-0.569, 1.272]

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.