ID	name	RMSE	MAE	ME	R^2	m
hdiyq	S+pKa	0.627 [0.461, 0.772]	0.478 [0.324, 0.638]	0.152 [-0.087, 0.379]	0.948 [0.909, 0.975]	1.038 [0.949, 1.162]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.427, 0.849]	0.495 [0.335, 0.672]	0.026 [-0.227, 0.290]	0.936 [0.851, 0.977]	0.978 [0.903, 1.053]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.457, 0.846]	0.520 [0.375, 0.688]	-0.089 [-0.341, 0.163]	0.943 [0.857, 0.981]	1.039 [0.968, 1.090]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.444, 0.908]	0.495 [0.322, 0.696]	0.058 [-0.208, 0.335]	0.924 [0.848, 0.972]	0.961 [0.848, 1.064]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.427, 0.970]	0.480 [0.295, 0.698]	0.159 [-0.095, 0.447]	0.920 [0.825, 0.975]	0.939 [0.833, 1.057]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.794 [0.480, 1.096]	0.577 [0.382, 0.816]	0.018 [-0.308, 0.315]	0.900 [0.747, 0.973]	0.899 [0.823, 0.971]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.618, 0.955]	0.639 [0.456, 0.825]	-0.243 [-0.534, 0.047]	0.911 [0.818, 0.958]	0.981 [0.825, 1.092]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.847 [0.549, 1.143]	0.631 [0.429, 0.868]	-0.091 [-0.423, 0.229]	0.923 [0.812, 0.976]	1.105 [1.016, 1.189]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.643, 1.157]	0.698 [0.478, 0.934]	0.276 [-0.069, 0.616]	0.892 [0.774, 0.955]	0.997 [0.877, 1.118]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.663, 1.187]	0.711 [0.495, 0.954]	0.172 [-0.170, 0.530]	0.870 [0.758, 0.937]	0.950 [0.815, 1.122]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.595, 1.347]	0.694 [0.458, 0.972]	-0.003 [-0.392, 0.353]	0.853 [0.658, 0.955]	0.920 [0.799, 1.011]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.721, 1.355]	0.766 [0.505, 1.047]	-0.409 [-0.786, -0.044]	0.915 [0.824, 0.964]	1.160 [0.996, 1.300]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.456, 1.666]	0.611 [0.324, 1.005]	0.126 [-0.246, 0.589]	0.892 [0.801, 0.975]	1.144 [0.966, 1.352]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.477, 1.673]	0.629 [0.337, 1.019]	0.085 [-0.293, 0.555]	0.892 [0.800, 0.974]	1.152 [0.968, 1.362]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.524, 1.653]	0.665 [0.395, 1.029]	0.238 [-0.126, 0.674]	0.851 [0.767, 0.954]	1.020 [0.821, 1.285]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.514, 1.688]	0.659 [0.376, 1.069]	0.225 [-0.146, 0.684]	0.858 [0.778, 0.959]	1.050 [0.843, 1.329]
arcko	Vertical scheme for type I submission	1.095 [0.751, 1.414]	0.815 [0.551, 1.114]	0.434 [0.055, 0.845]	0.865 [0.758, 0.933]	1.024 [0.896, 1.199]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.830, 1.348]	0.893 [0.655, 1.142]	0.440 [0.045, 0.817]	0.890 [0.760, 0.957]	1.112 [0.966, 1.253]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.523, 1.687]	0.675 [0.390, 1.063]	0.095 [-0.285, 0.565]	0.872 [0.790, 0.965]	1.118 [0.956, 1.363]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.781, 1.453]	0.863 [0.595, 1.160]	-0.367 [-0.785, 0.038]	0.895 [0.803, 0.949]	1.168 [1.024, 1.345]
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 [0.877, 1.493]	0.960 [0.704, 1.244]	0.331 [-0.104, 0.782]	0.862 [0.699, 0.942]	1.115 [0.959, 1.275]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.648, 1.810]	0.794 [0.462, 1.213]	0.132 [-0.320, 0.643]	0.861 [0.780, 0.952]	1.152 [0.977, 1.427]
6tvf8	OE Gaussian Process	1.326 [0.732, 1.795]	0.853 [0.480, 1.283]	0.156 [-0.350, 0.697]	0.598 [0.268, 0.868]	0.675 [0.395, 0.944]
v8qph	ACD/pKa GALAS	1.424 [0.883, 1.884]	1.019 [0.649, 1.443]	-0.065 [-0.642, 0.485]	0.841 [0.661, 0.942]	1.249 [0.994, 1.462]
wexjs	Direct scheme for type I submission	1.426 [1.060, 1.762]	1.154 [0.842, 1.493]	0.315 [-0.234, 0.876]	0.828 [0.636, 0.924]	1.187 [0.981, 1.408]
w4z0e	Direct scheme with single point correction for...	1.699 [1.270, 2.085]	1.390 [1.026, 1.782]	0.175 [-0.481, 0.807]	0.843 [0.728, 0.916]	1.353 [1.136, 1.637]
0wfzo	Explicit solvent submission 1	2.418 [1.320, 3.566]	1.610 [1.011, 2.401]	0.243 [-0.616, 1.272]	0.527 [0.265, 0.793]	1.080 [0.803, 1.492]
t8ewk	COSMOlogic_FINE17	2.799 [0.929, 4.027]	1.548 [0.694, 2.588]	0.865 [-0.118, 2.038]	0.097 [0.000, 0.817]	0.360 [-0.302, 1.043]
758j8	Explicit solvent submission 3	2.966 [1.893, 4.085]	2.204 [1.512, 3.087]	0.924 [-0.131, 2.080]	0.381 [0.111, 0.653]	0.942 [0.505, 1.417]
z3btx	Explicit solvent submission 2	3.506 [1.486, 5.334]	2.012 [1.040, 3.257]	1.357 [0.218, 2.754]	0.341 [0.154, 0.732]	0.993 [0.723, 1.412]
hgn83	Explicit solvent submission 4	4.519 [2.410, 6.282]	2.875 [1.583, 4.387]	1.417 [-0.211, 3.217]	0.214 [0.033, 0.540]	1.085 [0.550, 1.566]

Notes
- Mean and 95% confidence intervals of statistic values were calculated by bootstrapping.
- pKa predictions of Epik method (submission ID: nb00X) were not blind. They were submitted after the submission deadline to be used as a reference method.
pKas of the rest of the molecules in these submissions were blindly predicted before experimental data was released.