ID	name	RMSE	MAE	ME	R^2	m
hdiyq	S+pKa	0.624 [0.475, 0.756]	0.468 [0.328, 0.618]	0.127 [-0.095, 0.343]	0.950 [0.918, 0.974]	0.990 [0.916, 1.089]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.430, 0.810]	0.469 [0.324, 0.632]	-0.024 [-0.248, 0.204]	0.949 [0.892, 0.980]	0.982 [0.912, 1.045]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.469, 0.814]	0.499 [0.360, 0.651]	-0.099 [-0.327, 0.130]	0.948 [0.891, 0.978]	0.995 [0.924, 1.054]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.402, 0.888]	0.434 [0.270, 0.615]	0.113 [-0.106, 0.350]	0.941 [0.877, 0.981]	0.945 [0.868, 1.024]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.443, 0.859]	0.465 [0.311, 0.642]	0.003 [-0.227, 0.242]	0.940 [0.883, 0.977]	0.967 [0.871, 1.049]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.619, 0.934]	0.622 [0.455, 0.792]	-0.169 [-0.436, 0.109]	0.919 [0.866, 0.956]	0.948 [0.822, 1.057]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.583, 1.075]	0.613 [0.417, 0.826]	0.221 [-0.062, 0.514]	0.919 [0.838, 0.965]	0.999 [0.913, 1.088]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.609, 1.098]	0.621 [0.426, 0.849]	0.132 [-0.162, 0.439]	0.904 [0.825, 0.955]	0.961 [0.860, 1.081]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.504, 1.164]	0.588 [0.384, 0.829]	0.100 [-0.194, 0.416]	0.899 [0.774, 0.970]	0.917 [0.839, 0.979]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.561, 1.260]	0.615 [0.413, 0.865]	-0.025 [-0.353, 0.275]	0.892 [0.754, 0.964]	0.936 [0.853, 0.999]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.565, 1.325]	0.640 [0.415, 0.918]	0.003 [-0.319, 0.359]	0.900 [0.767, 0.973]	1.056 [0.960, 1.130]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.690, 1.271]	0.720 [0.499, 0.967]	-0.318 [-0.656, 0.001]	0.915 [0.857, 0.957]	1.089 [0.946, 1.223]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.446, 1.530]	0.561 [0.314, 0.890]	0.103 [-0.212, 0.490]	0.906 [0.828, 0.977]	1.089 [0.959, 1.255]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.473, 1.531]	0.574 [0.337, 0.896]	0.067 [-0.256, 0.452]	0.906 [0.826, 0.975]	1.096 [0.960, 1.255]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.753, 1.253]	0.782 [0.561, 1.018]	0.349 [0.017, 0.692]	0.906 [0.816, 0.956]	1.071 [0.964, 1.185]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.516, 1.539]	0.620 [0.385, 0.948]	0.188 [-0.130, 0.575]	0.878 [0.798, 0.964]	0.997 [0.844, 1.195]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.500, 1.537]	0.608 [0.367, 0.930]	0.083 [-0.240, 0.467]	0.896 [0.823, 0.972]	1.084 [0.969, 1.250]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.506, 1.555]	0.613 [0.369, 0.945]	0.168 [-0.161, 0.560]	0.883 [0.806, 0.966]	1.019 [0.866, 1.221]
arcko	Vertical scheme for type I submission	1.041 [0.730, 1.333]	0.767 [0.529, 1.034]	0.366 [0.032, 0.726]	0.886 [0.801, 0.942]	1.010 [0.904, 1.142]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.699, 1.336]	0.737 [0.489, 1.009]	-0.307 [-0.667, 0.028]	0.913 [0.848, 0.957]	1.125 [1.022, 1.258]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.801, 1.395]	0.841 [0.597, 1.109]	0.277 [-0.100, 0.665]	0.886 [0.778, 0.949]	1.094 [0.981, 1.220]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.605, 1.648]	0.696 [0.415, 1.043]	0.128 [-0.246, 0.555]	0.884 [0.812, 0.961]	1.103 [0.976, 1.283]
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 [0.491, 1.579]
wexjs	Direct scheme for type I submission	1.303 [0.958, 1.627]	0.978 [0.689, 1.295]	0.274 [-0.168, 0.732]	0.859 [0.735, 0.930]	1.134 [0.994, 1.288]
v8qph	ACD/pKa GALAS	1.373 [0.922, 1.778]	0.975 [0.654, 1.340]	-0.145 [-0.644, 0.334]	0.838 [0.702, 0.926]	1.147 [0.969, 1.324]
w4z0e	Direct scheme with single point correction for...	1.569 [1.173, 1.933]	1.226 [0.898, 1.580]	0.090 [-0.473, 0.631]	0.848 [0.763, 0.909]	1.246 [1.083, 1.456]
6tvf8	OE Gaussian Process	1.883 [0.870, 2.858]	1.023 [0.539, 1.671]	0.452 [-0.135, 1.163]	0.515 [0.152, 0.875]	0.584 [0.255, 0.890]
0wfzo	Explicit solvent submission 1	2.894 [1.732, 3.914]	1.880 [1.174, 2.719]	0.762 [-0.166, 1.799]	0.479 [0.215, 0.756]	0.995 [0.593, 1.383]
t8ewk	COSMOlogic_FINE17	3.300 [1.851, 4.410]	1.978 [1.050, 3.047]	1.317 [0.248, 2.521]	0.066 [0.000, 0.465]	0.253 [-0.171, 0.795]
z3btx	Explicit solvent submission 2	4.002 [2.292, 5.444]	2.486 [1.465, 3.660]	1.478 [0.241, 2.857]	0.287 [0.041, 0.607]	0.873 [0.303, 1.421]
758j8	Explicit solvent submission 3	4.524 [2.669, 6.156]	2.949 [1.877, 4.256]	1.846 [0.498, 3.380]	0.242 [0.016, 0.573]	0.864 [0.201, 1.515]
hgn83	Explicit solvent submission 4	6.375 [4.034, 8.446]	4.106 [2.510, 5.928]	2.131 [0.077, 4.255]	0.079 [0.000, 0.403]	0.647 [-0.184, 1.451]

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.