ID	name	RMSE	MAE	ME	R^2	m
hdiyq	S+pKa	0.627 [0.466, 0.776]	0.478 [0.329, 0.640]	0.152 [-0.087, 0.379]	0.948 [0.907, 0.975]	1.038 [0.948, 1.161]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.428, 0.849]	0.495 [0.335, 0.674]	0.026 [-0.233, 0.295]	0.936 [0.849, 0.977]	0.978 [0.902, 1.052]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.462, 0.843]	0.520 [0.375, 0.688]	-0.089 [-0.336, 0.164]	0.943 [0.860, 0.980]	1.039 [0.969, 1.091]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.445, 0.906]	0.495 [0.322, 0.692]	0.058 [-0.201, 0.334]	0.924 [0.847, 0.972]	0.961 [0.848, 1.064]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.422, 0.960]	0.480 [0.292, 0.694]	0.159 [-0.100, 0.438]	0.920 [0.820, 0.975]	0.939 [0.836, 1.055]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.794 [0.485, 1.095]	0.577 [0.385, 0.811]	0.018 [-0.295, 0.312]	0.900 [0.752, 0.972]	0.899 [0.822, 0.971]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.617, 0.954]	0.639 [0.457, 0.822]	-0.243 [-0.537, 0.047]	0.911 [0.818, 0.958]	0.981 [0.822, 1.092]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.847 [0.548, 1.138]	0.631 [0.425, 0.868]	-0.091 [-0.430, 0.237]	0.923 [0.813, 0.976]	1.105 [1.014, 1.191]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.641, 1.164]	0.698 [0.482, 0.936]	0.276 [-0.068, 0.622]	0.892 [0.772, 0.954]	0.997 [0.877, 1.122]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.666, 1.185]	0.711 [0.492, 0.958]	0.172 [-0.177, 0.528]	0.870 [0.758, 0.938]	0.950 [0.819, 1.119]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.594, 1.348]	0.694 [0.458, 0.978]	-0.003 [-0.383, 0.346]	0.853 [0.657, 0.955]	0.920 [0.798, 1.010]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.723, 1.361]	0.766 [0.510, 1.048]	-0.409 [-0.776, -0.045]	0.915 [0.826, 0.962]	1.160 [0.998, 1.298]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.463, 1.669]	0.611 [0.328, 1.008]	0.126 [-0.241, 0.592]	0.892 [0.806, 0.975]	1.144 [0.967, 1.354]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.483, 1.679]	0.629 [0.341, 1.022]	0.085 [-0.289, 0.556]	0.892 [0.799, 0.974]	1.152 [0.967, 1.369]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.523, 1.662]	0.665 [0.393, 1.047]	0.238 [-0.121, 0.687]	0.851 [0.768, 0.955]	1.020 [0.816, 1.285]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.512, 1.677]	0.659 [0.375, 1.045]	0.225 [-0.154, 0.688]	0.858 [0.781, 0.958]	1.050 [0.846, 1.324]
arcko	Vertical scheme for type I submission	1.095 [0.749, 1.410]	0.815 [0.546, 1.111]	0.434 [0.063, 0.832]	0.865 [0.758, 0.934]	1.024 [0.895, 1.200]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.833, 1.352]	0.893 [0.658, 1.148]	0.440 [0.048, 0.826]	0.890 [0.757, 0.957]	1.112 [0.966, 1.256]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.528, 1.682]	0.675 [0.398, 1.056]	0.095 [-0.285, 0.561]	0.872 [0.791, 0.963]	1.118 [0.959, 1.361]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.786, 1.445]	0.863 [0.597, 1.163]	-0.367 [-0.784, 0.038]	0.895 [0.804, 0.949]	1.168 [1.026, 1.342]
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 [0.865, 1.482]	0.960 [0.698, 1.238]	0.331 [-0.112, 0.779]	0.862 [0.705, 0.943]	1.115 [0.965, 1.276]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.654, 1.796]	0.794 [0.462, 1.205]	0.132 [-0.326, 0.655]	0.861 [0.780, 0.953]	1.152 [0.974, 1.415]
6tvf8	OE Gaussian Process	1.326 [0.732, 1.800]	0.853 [0.479, 1.286]	0.156 [-0.362, 0.694]	0.598 [0.268, 0.867]	0.675 [0.393, 0.950]
v8qph	ACD/pKa GALAS	1.424 [0.906, 1.874]	1.019 [0.655, 1.430]	-0.065 [-0.646, 0.493]	0.841 [0.669, 0.943]	1.249 [1.004, 1.459]
wexjs	Direct scheme for type I submission	1.426 [1.053, 1.761]	1.154 [0.830, 1.501]	0.315 [-0.226, 0.866]	0.828 [0.644, 0.925]	1.187 [0.985, 1.405]
w4z0e	Direct scheme with single point correction for...	1.699 [1.278, 2.085]	1.390 [1.030, 1.778]	0.175 [-0.487, 0.825]	0.843 [0.734, 0.914]	1.353 [1.139, 1.640]
0wfzo	Explicit solvent submission 1	2.418 [1.313, 3.585]	1.610 [1.000, 2.431]	0.243 [-0.623, 1.284]	0.527 [0.273, 0.795]	1.080 [0.806, 1.480]
t8ewk	COSMOlogic_FINE17	2.799 [0.918, 4.040]	1.548 [0.687, 2.596]	0.865 [-0.097, 2.063]	0.097 [0.000, 0.820]	0.360 [-0.317, 1.040]
758j8	Explicit solvent submission 3	2.966 [1.857, 4.037]	2.204 [1.486, 3.055]	0.924 [-0.106, 2.078]	0.381 [0.121, 0.663]	0.942 [0.520, 1.419]
z3btx	Explicit solvent submission 2	3.506 [1.483, 5.347]	2.012 [1.058, 3.276]	1.357 [0.230, 2.729]	0.341 [0.153, 0.726]	0.993 [0.725, 1.422]
hgn83	Explicit solvent submission 4	4.519 [2.393, 6.370]	2.875 [1.587, 4.435]	1.417 [-0.208, 3.261]	0.214 [0.036, 0.538]	1.085 [0.543, 1.567]

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.