ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.301, 0.641]	0.329 [0.222, 0.455]	-0.019 [-0.188, 0.141]	0.971 [0.936, 0.990]	1.010 [0.965, 1.059]
hdiyq	S+pKa	0.607 [0.451, 0.743]	0.450 [0.308, 0.599]	0.098 [-0.114, 0.311]	0.950 [0.913, 0.975]	1.011 [0.933, 1.110]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.435, 0.812]	0.469 [0.324, 0.633]	-0.024 [-0.249, 0.212]	0.949 [0.889, 0.980]	0.982 [0.910, 1.045]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.462, 0.818]	0.499 [0.357, 0.655]	-0.099 [-0.325, 0.132]	0.948 [0.889, 0.979]	0.995 [0.925, 1.056]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.663 [0.410, 0.907]	0.443 [0.279, 0.638]	0.111 [-0.113, 0.361]	0.938 [0.862, 0.979]	0.943 [0.857, 1.029]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.439, 0.859]	0.465 [0.308, 0.639]	0.003 [-0.227, 0.242]	0.940 [0.885, 0.977]	0.967 [0.871, 1.049]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.723 [0.419, 1.002]	0.504 [0.331, 0.708]	-0.017 [-0.297, 0.238]	0.925 [0.818, 0.979]	0.949 [0.889, 1.002]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.760 [0.594, 0.909]	0.596 [0.433, 0.767]	-0.221 [-0.477, 0.034]	0.924 [0.851, 0.962]	0.982 [0.858, 1.074]
nb008	Epik Microscopic	0.761 [0.491, 1.024]	0.523 [0.346, 0.737]	-0.084 [-0.369, 0.172]	0.930 [0.847, 0.976]	0.853 [0.784, 0.925]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.781 [0.508, 1.054]	0.555 [0.375, 0.763]	-0.104 [-0.387, 0.173]	0.940 [0.863, 0.980]	1.077 [1.013, 1.141]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.590, 1.086]	0.633 [0.436, 0.850]	0.230 [-0.065, 0.525]	0.914 [0.822, 0.963]	0.994 [0.906, 1.090]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.608, 1.099]	0.621 [0.423, 0.842]	0.132 [-0.155, 0.436]	0.904 [0.824, 0.954]	0.961 [0.858, 1.076]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.561, 1.245]	0.615 [0.413, 0.862]	-0.025 [-0.342, 0.278]	0.892 [0.758, 0.964]	0.936 [0.854, 1.000]
nb016	MoKa	0.952 [0.709, 1.183]	0.767 [0.567, 0.986]	-0.225 [-0.570, 0.117]	0.895 [0.823, 0.947]	0.935 [0.819, 1.069]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.687, 1.275]	0.720 [0.495, 0.968]	-0.318 [-0.655, -0.009]	0.915 [0.856, 0.957]	1.089 [0.947, 1.221]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.449, 1.540]	0.561 [0.320, 0.899]	0.103 [-0.209, 0.490]	0.906 [0.826, 0.977]	1.089 [0.956, 1.255]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.468, 1.535]	0.574 [0.330, 0.912]	0.067 [-0.250, 0.460]	0.906 [0.829, 0.975]	1.096 [0.960, 1.264]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.750, 1.245]	0.782 [0.557, 1.011]	0.349 [0.011, 0.689]	0.906 [0.817, 0.956]	1.071 [0.964, 1.183]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.514, 1.543]	0.620 [0.384, 0.949]	0.188 [-0.128, 0.568]	0.878 [0.797, 0.964]	0.997 [0.846, 1.192]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.494, 1.543]	0.608 [0.363, 0.931]	0.083 [-0.237, 0.470]	0.896 [0.822, 0.972]	1.084 [0.968, 1.256]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.509, 1.549]	0.613 [0.369, 0.940]	0.168 [-0.152, 0.568]	0.883 [0.809, 0.964]	1.019 [0.868, 1.219]
arcko	Vertical scheme for type I submission	1.041 [0.738, 1.329]	0.767 [0.532, 1.030]	0.366 [0.039, 0.717]	0.886 [0.799, 0.943]	1.010 [0.902, 1.140]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.710, 1.333]	0.737 [0.493, 1.005]	-0.307 [-0.669, 0.035]	0.913 [0.848, 0.956]	1.125 [1.023, 1.257]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.804, 1.392]	0.841 [0.597, 1.109]	0.277 [-0.098, 0.668]	0.886 [0.771, 0.949]	1.094 [0.978, 1.222]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.604, 1.669]	0.696 [0.414, 1.060]	0.128 [-0.254, 0.563]	0.884 [0.811, 0.961]	1.103 [0.977, 1.292]
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]
6tvf8	OE Gaussian Process	1.251 [0.733, 1.685]	0.789 [0.464, 1.173]	0.199 [-0.239, 0.653]	0.736 [0.476, 0.912]	0.762 [0.551, 0.933]
v8qph	ACD/pKa GALAS	1.314 [0.839, 1.747]	0.921 [0.603, 1.298]	-0.062 [-0.558, 0.404]	0.859 [0.738, 0.938]	1.163 [0.987, 1.341]
wexjs	Direct scheme for type I submission	1.325 [0.969, 1.647]	1.009 [0.709, 1.327]	0.281 [-0.174, 0.759]	0.847 [0.707, 0.926]	1.146 [0.989, 1.314]
w4z0e	Direct scheme with single point correction for...	1.569 [1.177, 1.949]	1.226 [0.902, 1.588]	0.090 [-0.480, 0.640]	0.848 [0.765, 0.909]	1.246 [1.085, 1.467]
t8ewk	COSMOlogic_FINE17	2.685 [0.913, 3.884]	1.437 [0.662, 2.425]	0.808 [-0.071, 1.896]	0.130 [0.000, 0.822]	0.408 [-0.210, 1.047]
758j8	Explicit solvent submission 3	4.301 [2.138, 6.432]	2.650 [1.618, 3.997]	0.339 [-1.344, 1.730]	0.258 [0.071, 0.670]	0.972 [0.635, 1.343]
z3btx	Explicit solvent submission 2	4.825 [1.881, 7.315]	2.528 [1.273, 4.163]	0.554 [-1.337, 2.172]	0.247 [0.076, 0.721]	1.057 [0.745, 1.385]
0wfzo	Explicit solvent submission 1	4.972 [1.391, 8.144]	2.237 [1.027, 4.084]	-0.638 [-2.688, 0.821]	0.196 [0.049, 0.782]	0.990 [0.705, 1.294]
hgn83	Explicit solvent submission 4	5.111 [3.052, 6.814]	3.207 [1.814, 4.784]	1.006 [-0.835, 2.894]	0.271 [0.099, 0.554]	1.254 [0.865, 1.724]

Notes
- In this analysis we assumed well separated experimental macroscopic pKas represent microscopic pKas. Molecules with experimental pKa values at least 3 units apart were considered well-separated. SM14 and SM18 which do not satify this criteria are ignored in this analysis.
- Mean and 95% confidence intervals of statistic values were calculated by bootstrapping.
- pKa predictions of Epik, Jaguar, Chemicalize, and MoKa were not blind (submission IDs noted as nbXXX). They were submitted after the submission deadline as reference methods.
- pKas of the rest of the molecules in these submissions were blindly predicted before experimental data was released.