ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.299, 0.627]	0.329 [0.215, 0.445]	-0.019 [-0.181, 0.139]	0.971 [0.941, 0.990]	1.010 [0.967, 1.066]
hdiyq	S+pKa	0.607 [0.449, 0.738]	0.450 [0.302, 0.601]	0.098 [-0.104, 0.314]	0.950 [0.912, 0.977]	1.011 [0.931, 1.124]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.438, 0.812]	0.469 [0.328, 0.634]	-0.024 [-0.261, 0.200]	0.949 [0.887, 0.980]	0.982 [0.914, 1.043]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.463, 0.838]	0.499 [0.364, 0.663]	-0.099 [-0.346, 0.134]	0.948 [0.885, 0.979]	0.995 [0.919, 1.052]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.663 [0.406, 0.900]	0.443 [0.280, 0.639]	0.111 [-0.126, 0.350]	0.938 [0.866, 0.981]	0.943 [0.855, 1.038]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.448, 0.862]	0.465 [0.304, 0.652]	0.003 [-0.225, 0.265]	0.940 [0.888, 0.979]	0.967 [0.878, 1.048]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.723 [0.429, 1.011]	0.504 [0.340, 0.714]	-0.017 [-0.296, 0.240]	0.925 [0.813, 0.981]	0.949 [0.891, 1.006]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.760 [0.588, 0.909]	0.596 [0.424, 0.767]	-0.221 [-0.475, 0.058]	0.924 [0.850, 0.963]	0.982 [0.850, 1.075]
nb008	Epik Microscopic	0.761 [0.476, 1.027]	0.523 [0.330, 0.739]	-0.084 [-0.364, 0.178]	0.930 [0.847, 0.977]	0.853 [0.782, 0.923]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.781 [0.504, 1.060]	0.555 [0.377, 0.771]	-0.104 [-0.371, 0.192]	0.940 [0.859, 0.979]	1.077 [1.017, 1.149]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.587, 1.105]	0.633 [0.434, 0.852]	0.230 [-0.058, 0.572]	0.914 [0.825, 0.963]	0.994 [0.905, 1.098]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.596, 1.106]	0.621 [0.421, 0.847]	0.132 [-0.180, 0.433]	0.904 [0.816, 0.958]	0.961 [0.858, 1.073]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.543, 1.279]	0.615 [0.399, 0.881]	-0.025 [-0.349, 0.288]	0.892 [0.751, 0.967]	0.936 [0.853, 1.008]
nb016	MoKa	0.952 [0.701, 1.167]	0.767 [0.565, 0.975]	-0.225 [-0.557, 0.121]	0.895 [0.834, 0.947]	0.935 [0.813, 1.071]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.704, 1.257]	0.720 [0.500, 0.961]	-0.318 [-0.636, -0.015]	0.915 [0.851, 0.959]	1.089 [0.943, 1.232]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.447, 1.556]	0.561 [0.319, 0.910]	0.103 [-0.201, 0.528]	0.906 [0.830, 0.977]	1.089 [0.955, 1.263]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.476, 1.566]	0.574 [0.334, 0.930]	0.067 [-0.250, 0.455]	0.906 [0.828, 0.977]	1.096 [0.964, 1.273]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.761, 1.246]	0.782 [0.559, 1.019]	0.349 [0.035, 0.682]	0.906 [0.807, 0.956]	1.071 [0.950, 1.195]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.508, 1.508]	0.620 [0.379, 0.917]	0.188 [-0.115, 0.553]	0.878 [0.798, 0.964]	0.997 [0.850, 1.188]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.498, 1.626]	0.608 [0.356, 0.962]	0.083 [-0.257, 0.485]	0.896 [0.817, 0.973]	1.084 [0.968, 1.271]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.515, 1.540]	0.613 [0.365, 0.945]	0.168 [-0.156, 0.592]	0.883 [0.796, 0.966]	1.019 [0.860, 1.214]
arcko	Vertical scheme for type I submission	1.041 [0.743, 1.333]	0.767 [0.541, 1.019]	0.366 [0.031, 0.727]	0.886 [0.810, 0.943]	1.010 [0.908, 1.142]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.713, 1.354]	0.737 [0.497, 1.015]	-0.307 [-0.659, 0.067]	0.913 [0.846, 0.956]	1.125 [1.022, 1.258]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.817, 1.427]	0.841 [0.604, 1.129]	0.277 [-0.077, 0.687]	0.886 [0.774, 0.950]	1.094 [0.983, 1.222]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.573, 1.683]	0.696 [0.390, 1.052]	0.128 [-0.223, 0.555]	0.884 [0.809, 0.962]	1.103 [0.974, 1.321]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.296, 1.660]	0.884 [0.228, 1.576]	-0.764 [-1.540, 0.012]	0.914 [0.457, 1.000]	1.162 [0.519, 2.305]
6tvf8	OE Gaussian Process	1.251 [0.707, 1.660]	0.789 [0.450, 1.158]	0.199 [-0.223, 0.672]	0.736 [0.472, 0.914]	0.762 [0.551, 0.943]
v8qph	ACD/pKa GALAS	1.314 [0.823, 1.737]	0.921 [0.600, 1.301]	-0.062 [-0.547, 0.388]	0.859 [0.737, 0.941]	1.163 [0.983, 1.344]
wexjs	Direct scheme for type I submission	1.325 [0.979, 1.648]	1.009 [0.721, 1.342]	0.281 [-0.184, 0.780]	0.847 [0.687, 0.928]	1.146 [0.977, 1.334]
w4z0e	Direct scheme with single point correction for...	1.569 [1.173, 1.955]	1.226 [0.878, 1.609]	0.090 [-0.449, 0.655]	0.848 [0.766, 0.911]	1.246 [1.083, 1.463]
t8ewk	COSMOlogic_FINE17	2.685 [0.845, 3.925]	1.437 [0.617, 2.468]	0.808 [-0.124, 1.870]	0.130 [0.000, 0.865]	0.408 [-0.252, 1.076]
758j8	Explicit solvent submission 3	4.301 [2.229, 6.349]	2.650 [1.676, 4.031]	0.339 [-1.244, 1.778]	0.258 [0.078, 0.657]	0.972 [0.639, 1.389]
z3btx	Explicit solvent submission 2	4.825 [1.917, 7.253]	2.528 [1.311, 4.144]	0.554 [-1.231, 2.052]	0.247 [0.071, 0.726]	1.057 [0.741, 1.384]
0wfzo	Explicit solvent submission 1	4.972 [1.403, 9.002]	2.237 [1.014, 4.417]	-0.638 [-2.929, 0.855]	0.196 [0.048, 0.793]	0.990 [0.709, 1.359]
hgn83	Explicit solvent submission 4	5.111 [3.154, 6.883]	3.207 [1.861, 4.870]	1.006 [-0.842, 2.836]	0.271 [0.091, 0.549]	1.254 [0.862, 1.746]

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.