ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.304, 0.651]	0.329 [0.227, 0.458]	-0.019 [-0.185, 0.145]	0.971 [0.935, 0.990]	1.010 [0.969, 1.061]
hdiyq	S+pKa	0.607 [0.441, 0.751]	0.450 [0.296, 0.609]	0.098 [-0.129, 0.294]	0.950 [0.913, 0.976]	1.011 [0.935, 1.114]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.440, 0.816]	0.469 [0.326, 0.624]	-0.024 [-0.261, 0.194]	0.949 [0.894, 0.981]	0.982 [0.914, 1.052]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.474, 0.826]	0.499 [0.360, 0.667]	-0.099 [-0.318, 0.153]	0.948 [0.887, 0.979]	0.995 [0.916, 1.054]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.663 [0.421, 0.913]	0.443 [0.288, 0.648]	0.111 [-0.111, 0.356]	0.938 [0.868, 0.979]	0.943 [0.856, 1.035]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.448, 0.870]	0.465 [0.315, 0.654]	0.003 [-0.224, 0.249]	0.940 [0.876, 0.977]	0.967 [0.863, 1.051]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.723 [0.422, 1.003]	0.504 [0.341, 0.714]	-0.017 [-0.305, 0.248]	0.925 [0.814, 0.981]	0.949 [0.885, 1.005]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.760 [0.583, 0.907]	0.596 [0.430, 0.760]	-0.221 [-0.474, 0.074]	0.924 [0.852, 0.961]	0.982 [0.858, 1.073]
nb008	Epik Microscopic	0.761 [0.484, 1.053]	0.523 [0.336, 0.769]	-0.084 [-0.361, 0.164]	0.930 [0.849, 0.978]	0.853 [0.781, 0.932]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.781 [0.518, 1.054]	0.555 [0.376, 0.772]	-0.104 [-0.378, 0.156]	0.940 [0.866, 0.980]	1.077 [1.009, 1.146]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.585, 1.087]	0.633 [0.425, 0.848]	0.230 [-0.069, 0.513]	0.914 [0.828, 0.965]	0.994 [0.906, 1.090]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.607, 1.084]	0.621 [0.425, 0.834]	0.132 [-0.149, 0.429]	0.904 [0.831, 0.957]	0.961 [0.864, 1.083]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.556, 1.263]	0.615 [0.407, 0.865]	-0.025 [-0.340, 0.286]	0.892 [0.737, 0.966]	0.936 [0.849, 1.006]
nb016	MoKa	0.952 [0.718, 1.190]	0.767 [0.572, 0.998]	-0.225 [-0.564, 0.108]	0.895 [0.824, 0.948]	0.935 [0.829, 1.068]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.693, 1.283]	0.720 [0.501, 0.988]	-0.318 [-0.669, -0.007]	0.915 [0.860, 0.959]	1.089 [0.941, 1.233]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.456, 1.537]	0.561 [0.316, 0.891]	0.103 [-0.197, 0.502]	0.906 [0.833, 0.977]	1.089 [0.959, 1.257]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.475, 1.594]	0.574 [0.341, 0.897]	0.067 [-0.270, 0.472]	0.906 [0.824, 0.975]	1.096 [0.959, 1.263]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.758, 1.243]	0.782 [0.566, 1.007]	0.349 [0.031, 0.701]	0.906 [0.818, 0.957]	1.071 [0.967, 1.187]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.517, 1.566]	0.620 [0.384, 0.962]	0.188 [-0.134, 0.564]	0.878 [0.802, 0.965]	0.997 [0.847, 1.183]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.498, 1.548]	0.613 [0.362, 0.965]	0.168 [-0.155, 0.570]	0.883 [0.806, 0.967]	1.019 [0.861, 1.226]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.506, 1.579]	0.608 [0.363, 0.968]	0.083 [-0.232, 0.468]	0.896 [0.820, 0.971]	1.084 [0.969, 1.267]
arcko	Vertical scheme for type I submission	1.041 [0.756, 1.339]	0.767 [0.540, 1.039]	0.366 [0.041, 0.756]	0.886 [0.803, 0.944]	1.010 [0.903, 1.146]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.710, 1.354]	0.737 [0.485, 1.007]	-0.307 [-0.670, 0.044]	0.913 [0.850, 0.957]	1.125 [1.024, 1.266]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.795, 1.409]	0.841 [0.593, 1.102]	0.277 [-0.082, 0.717]	0.886 [0.775, 0.949]	1.094 [0.981, 1.227]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.604, 1.660]	0.696 [0.419, 1.063]	0.128 [-0.249, 0.553]	0.884 [0.807, 0.962]	1.103 [0.979, 1.302]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.296, 1.647]	0.884 [0.228, 1.540]	-0.764 [-1.540, 0.030]	0.914 [0.457, 1.000]	1.162 [0.519, 1.592]
6tvf8	OE Gaussian Process	1.251 [0.736, 1.701]	0.789 [0.468, 1.175]	0.199 [-0.243, 0.665]	0.736 [0.469, 0.909]	0.762 [0.554, 0.932]
v8qph	ACD/pKa GALAS	1.314 [0.877, 1.749]	0.921 [0.619, 1.308]	-0.062 [-0.542, 0.435]	0.859 [0.726, 0.938]	1.163 [0.985, 1.338]
wexjs	Direct scheme for type I submission	1.325 [0.978, 1.673]	1.009 [0.699, 1.354]	0.281 [-0.161, 0.724]	0.847 [0.697, 0.923]	1.146 [0.993, 1.326]
w4z0e	Direct scheme with single point correction for...	1.569 [1.176, 1.949]	1.226 [0.887, 1.600]	0.090 [-0.463, 0.646]	0.848 [0.768, 0.910]	1.246 [1.074, 1.460]
t8ewk	COSMOlogic_FINE17	2.685 [0.854, 3.941]	1.437 [0.628, 2.462]	0.808 [-0.097, 1.931]	0.130 [0.001, 0.846]	0.408 [-0.247, 1.050]
758j8	Explicit solvent submission 3	4.301 [2.160, 6.590]	2.650 [1.632, 4.094]	0.339 [-1.427, 1.812]	0.258 [0.064, 0.667]	0.972 [0.627, 1.374]
z3btx	Explicit solvent submission 2	4.825 [1.933, 7.621]	2.528 [1.262, 4.423]	0.554 [-1.258, 2.160]	0.247 [0.077, 0.713]	1.057 [0.745, 1.401]
0wfzo	Explicit solvent submission 1	4.972 [1.319, 8.203]	2.237 [0.981, 4.189]	-0.638 [-2.594, 0.769]	0.196 [0.043, 0.797]	0.990 [0.689, 1.287]
hgn83	Explicit solvent submission 4	5.111 [3.044, 6.793]	3.207 [1.786, 4.765]	1.006 [-0.869, 2.901]	0.271 [0.094, 0.573]	1.254 [0.868, 1.725]

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.