ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.300, 0.644]	0.329 [0.223, 0.459]	-0.019 [-0.193, 0.139]	0.971 [0.935, 0.990]	1.010 [0.967, 1.061]
hdiyq	S+pKa	0.607 [0.455, 0.742]	0.450 [0.310, 0.600]	0.098 [-0.115, 0.311]	0.950 [0.912, 0.975]	1.011 [0.934, 1.112]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.433, 0.807]	0.469 [0.324, 0.632]	-0.024 [-0.257, 0.211]	0.949 [0.891, 0.980]	0.982 [0.913, 1.044]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.463, 0.813]	0.499 [0.358, 0.649]	-0.099 [-0.330, 0.128]	0.948 [0.889, 0.978]	0.995 [0.923, 1.057]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.663 [0.412, 0.908]	0.443 [0.279, 0.638]	0.111 [-0.114, 0.359]	0.938 [0.863, 0.979]	0.943 [0.854, 1.028]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.440, 0.860]	0.465 [0.310, 0.644]	0.003 [-0.226, 0.247]	0.940 [0.885, 0.977]	0.967 [0.869, 1.049]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.723 [0.419, 1.006]	0.504 [0.334, 0.714]	-0.017 [-0.280, 0.241]	0.925 [0.815, 0.979]	0.949 [0.889, 1.003]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.760 [0.593, 0.906]	0.596 [0.433, 0.766]	-0.221 [-0.479, 0.042]	0.924 [0.855, 0.961]	0.982 [0.858, 1.074]
nb008	Epik Microscopic	0.761 [0.482, 1.015]	0.523 [0.339, 0.734]	-0.084 [-0.363, 0.172]	0.930 [0.847, 0.977]	0.853 [0.786, 0.927]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.781 [0.508, 1.053]	0.555 [0.376, 0.766]	-0.104 [-0.384, 0.175]	0.940 [0.864, 0.979]	1.077 [1.014, 1.142]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.592, 1.090]	0.633 [0.434, 0.851]	0.230 [-0.070, 0.534]	0.914 [0.827, 0.963]	0.994 [0.906, 1.087]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.603, 1.093]	0.621 [0.424, 0.839]	0.132 [-0.160, 0.437]	0.904 [0.824, 0.955]	0.961 [0.859, 1.078]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.556, 1.247]	0.615 [0.411, 0.864]	-0.025 [-0.350, 0.278]	0.892 [0.755, 0.965]	0.936 [0.852, 1.003]
nb016	MoKa	0.952 [0.709, 1.173]	0.767 [0.568, 0.983]	-0.225 [-0.570, 0.116]	0.895 [0.824, 0.945]	0.935 [0.821, 1.073]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.691, 1.262]	0.720 [0.500, 0.963]	-0.318 [-0.648, -0.003]	0.915 [0.859, 0.957]	1.089 [0.947, 1.219]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.448, 1.530]	0.561 [0.319, 0.890]	0.103 [-0.207, 0.492]	0.906 [0.828, 0.977]	1.089 [0.957, 1.255]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.467, 1.533]	0.574 [0.330, 0.900]	0.067 [-0.254, 0.455]	0.906 [0.828, 0.977]	1.096 [0.962, 1.257]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.759, 1.255]	0.782 [0.566, 1.019]	0.349 [0.021, 0.685]	0.906 [0.816, 0.956]	1.071 [0.959, 1.186]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.513, 1.539]	0.620 [0.381, 0.945]	0.188 [-0.120, 0.579]	0.878 [0.800, 0.964]	0.997 [0.845, 1.191]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.502, 1.545]	0.608 [0.367, 0.934]	0.083 [-0.241, 0.475]	0.896 [0.821, 0.971]	1.084 [0.968, 1.252]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.513, 1.554]	0.613 [0.371, 0.951]	0.168 [-0.154, 0.561]	0.883 [0.804, 0.965]	1.019 [0.866, 1.218]
arcko	Vertical scheme for type I submission	1.041 [0.728, 1.327]	0.767 [0.528, 1.034]	0.366 [0.032, 0.716]	0.886 [0.800, 0.942]	1.010 [0.901, 1.143]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.701, 1.340]	0.737 [0.495, 1.009]	-0.307 [-0.666, 0.036]	0.913 [0.849, 0.957]	1.125 [1.022, 1.259]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.804, 1.401]	0.841 [0.596, 1.114]	0.277 [-0.092, 0.665]	0.886 [0.776, 0.948]	1.094 [0.981, 1.223]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.604, 1.650]	0.696 [0.412, 1.047]	0.128 [-0.241, 0.567]	0.884 [0.811, 0.961]	1.103 [0.974, 1.291]
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 [0.726, 1.680]	0.789 [0.457, 1.169]	0.199 [-0.238, 0.661]	0.736 [0.480, 0.910]	0.762 [0.548, 0.932]
v8qph	ACD/pKa GALAS	1.314 [0.840, 1.736]	0.921 [0.608, 1.283]	-0.062 [-0.542, 0.408]	0.859 [0.737, 0.939]	1.163 [0.987, 1.339]
wexjs	Direct scheme for type I submission	1.325 [0.968, 1.650]	1.009 [0.708, 1.330]	0.281 [-0.178, 0.760]	0.847 [0.704, 0.925]	1.146 [0.992, 1.310]
w4z0e	Direct scheme with single point correction for...	1.569 [1.166, 1.926]	1.226 [0.891, 1.579]	0.090 [-0.473, 0.633]	0.848 [0.761, 0.909]	1.246 [1.084, 1.455]
t8ewk	COSMOlogic_FINE17	2.685 [0.886, 3.882]	1.437 [0.648, 2.413]	0.808 [-0.095, 1.910]	0.130 [0.000, 0.837]	0.408 [-0.205, 1.048]
758j8	Explicit solvent submission 3	4.301 [2.141, 6.502]	2.650 [1.627, 4.015]	0.339 [-1.390, 1.778]	0.258 [0.073, 0.667]	0.972 [0.633, 1.362]
z3btx	Explicit solvent submission 2	4.825 [1.870, 7.353]	2.528 [1.268, 4.192]	0.554 [-1.320, 2.121]	0.247 [0.074, 0.734]	1.057 [0.743, 1.387]
0wfzo	Explicit solvent submission 1	4.972 [1.399, 8.166]	2.237 [1.023, 4.120]	-0.638 [-2.662, 0.877]	0.196 [0.050, 0.783]	0.990 [0.705, 1.308]
hgn83	Explicit solvent submission 4	5.111 [3.122, 6.809]	3.207 [1.869, 4.775]	1.006 [-0.838, 2.883]	0.271 [0.095, 0.558]	1.254 [0.866, 1.708]

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.