ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.300, 0.648]	0.329 [0.221, 0.460]	-0.019 [-0.195, 0.143]	0.971 [0.936, 0.990]	1.010 [0.963, 1.062]
hdiyq	S+pKa	0.624 [0.472, 0.769]	0.468 [0.322, 0.638]	0.127 [-0.090, 0.351]	0.950 [0.919, 0.976]	0.990 [0.912, 1.091]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.431, 0.821]	0.469 [0.322, 0.640]	-0.024 [-0.249, 0.223]	0.949 [0.890, 0.980]	0.982 [0.917, 1.051]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.455, 0.838]	0.499 [0.350, 0.671]	-0.099 [-0.327, 0.128]	0.948 [0.883, 0.981]	0.995 [0.925, 1.059]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.393, 0.898]	0.434 [0.274, 0.621]	0.113 [-0.101, 0.373]	0.941 [0.876, 0.981]	0.945 [0.872, 1.023]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.437, 0.850]	0.465 [0.311, 0.635]	0.003 [-0.198, 0.249]	0.940 [0.884, 0.977]	0.967 [0.867, 1.048]
nb008	Epik Microscopic	0.761 [0.467, 1.036]	0.523 [0.324, 0.755]	-0.084 [-0.365, 0.176]	0.930 [0.848, 0.978]	0.853 [0.787, 0.927]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.625, 0.937]	0.622 [0.461, 0.787]	-0.169 [-0.439, 0.128]	0.919 [0.864, 0.957]	0.948 [0.824, 1.061]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.582, 1.060]	0.613 [0.427, 0.829]	0.221 [-0.075, 0.513]	0.919 [0.845, 0.964]	0.999 [0.908, 1.091]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.607, 1.098]	0.621 [0.420, 0.859]	0.132 [-0.133, 0.455]	0.904 [0.819, 0.957]	0.961 [0.860, 1.078]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.516, 1.182]	0.588 [0.388, 0.840]	0.100 [-0.202, 0.422]	0.899 [0.776, 0.968]	0.917 [0.837, 0.977]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.541, 1.238]	0.615 [0.397, 0.864]	-0.025 [-0.339, 0.293]	0.892 [0.762, 0.968]	0.936 [0.843, 1.006]
nb016	MoKa	0.952 [0.698, 1.177]	0.767 [0.569, 0.986]	-0.225 [-0.599, 0.143]	0.895 [0.823, 0.950]	0.935 [0.826, 1.083]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.570, 1.347]	0.640 [0.418, 0.925]	0.003 [-0.345, 0.342]	0.900 [0.771, 0.972]	1.056 [0.963, 1.132]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.673, 1.283]	0.720 [0.485, 0.981]	-0.318 [-0.643, -0.007]	0.915 [0.852, 0.957]	1.089 [0.958, 1.231]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.455, 1.524]	0.561 [0.335, 0.896]	0.103 [-0.213, 0.489]	0.906 [0.839, 0.976]	1.089 [0.963, 1.237]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.465, 1.562]	0.574 [0.333, 0.919]	0.067 [-0.246, 0.457]	0.906 [0.828, 0.978]	1.096 [0.958, 1.266]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.759, 1.247]	0.782 [0.570, 1.018]	0.349 [0.013, 0.685]	0.906 [0.818, 0.955]	1.071 [0.962, 1.188]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.510, 1.576]	0.620 [0.386, 0.947]	0.188 [-0.122, 0.575]	0.878 [0.801, 0.965]	0.997 [0.844, 1.194]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.478, 1.570]	0.608 [0.359, 0.925]	0.083 [-0.254, 0.463]	0.896 [0.824, 0.974]	1.084 [0.970, 1.261]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.499, 1.629]	0.613 [0.359, 0.989]	0.168 [-0.160, 0.608]	0.883 [0.803, 0.966]	1.019 [0.864, 1.222]
arcko	Vertical scheme for type I submission	1.041 [0.732, 1.325]	0.767 [0.519, 1.024]	0.366 [0.028, 0.744]	0.886 [0.808, 0.943]	1.010 [0.905, 1.142]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.711, 1.358]	0.737 [0.504, 1.030]	-0.307 [-0.648, 0.048]	0.913 [0.842, 0.959]	1.125 [1.024, 1.269]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.796, 1.370]	0.841 [0.579, 1.090]	0.277 [-0.131, 0.657]	0.886 [0.775, 0.951]	1.094 [0.984, 1.224]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.584, 1.674]	0.696 [0.407, 1.066]	0.128 [-0.251, 0.562]	0.884 [0.810, 0.964]	1.103 [0.970, 1.295]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.296, 1.660]	0.884 [0.228, 1.540]	-0.764 [-1.540, 0.060]	0.914 [0.457, 1.000]	1.162 [0.519, 1.592]
wexjs	Direct scheme for type I submission	1.303 [0.948, 1.642]	0.978 [0.679, 1.312]	0.274 [-0.167, 0.755]	0.859 [0.725, 0.934]	1.134 [0.975, 1.314]
v8qph	ACD/pKa GALAS	1.373 [0.947, 1.799]	0.975 [0.652, 1.371]	-0.145 [-0.619, 0.369]	0.838 [0.694, 0.924]	1.147 [0.960, 1.320]
w4z0e	Direct scheme with single point correction for...	1.569 [1.160, 1.932]	1.226 [0.889, 1.583]	0.090 [-0.478, 0.637]	0.848 [0.767, 0.912]	1.246 [1.080, 1.450]
6tvf8	OE Gaussian Process	1.883 [0.856, 2.907]	1.023 [0.529, 1.694]	0.452 [-0.142, 1.201]	0.515 [0.161, 0.888]	0.584 [0.271, 0.908]
0wfzo	Explicit solvent submission 1	2.894 [1.820, 3.978]	1.880 [1.195, 2.773]	0.762 [-0.273, 1.878]	0.479 [0.198, 0.743]	0.995 [0.606, 1.410]
t8ewk	COSMOlogic_FINE17	3.300 [2.014, 4.371]	1.978 [1.115, 3.006]	1.317 [0.250, 2.444]	0.066 [0.000, 0.393]	0.253 [-0.177, 0.734]
z3btx	Explicit solvent submission 2	4.002 [2.161, 5.587]	2.486 [1.439, 3.740]	1.478 [0.214, 2.973]	0.287 [0.044, 0.629]	0.873 [0.297, 1.461]
758j8	Explicit solvent submission 3	4.524 [2.431, 6.174]	2.949 [1.750, 4.267]	1.846 [0.338, 3.358]	0.242 [0.007, 0.582]	0.864 [0.145, 1.523]
hgn83	Explicit solvent submission 4	6.375 [4.036, 8.506]	4.106 [2.586, 6.074]	2.131 [0.075, 4.561]	0.079 [0.000, 0.419]	0.647 [-0.181, 1.523]

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.