ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.300, 0.640]	0.329 [0.221, 0.459]	-0.019 [-0.189, 0.142]	0.971 [0.936, 0.990]	1.010 [0.966, 1.061]
hdiyq	S+pKa	0.624 [0.476, 0.757]	0.468 [0.328, 0.618]	0.127 [-0.088, 0.340]	0.950 [0.918, 0.974]	0.990 [0.917, 1.088]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.437, 0.806]	0.469 [0.326, 0.631]	-0.024 [-0.250, 0.214]	0.949 [0.891, 0.980]	0.982 [0.911, 1.046]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.467, 0.813]	0.499 [0.359, 0.651]	-0.099 [-0.326, 0.130]	0.948 [0.889, 0.978]	0.995 [0.922, 1.055]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.402, 0.890]	0.434 [0.273, 0.622]	0.113 [-0.109, 0.349]	0.941 [0.874, 0.980]	0.945 [0.867, 1.024]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.438, 0.861]	0.465 [0.309, 0.645]	0.003 [-0.220, 0.241]	0.940 [0.885, 0.977]	0.967 [0.870, 1.049]
nb008	Epik Microscopic	0.761 [0.483, 1.014]	0.523 [0.341, 0.734]	-0.084 [-0.358, 0.173]	0.930 [0.848, 0.976]	0.853 [0.785, 0.925]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.622, 0.934]	0.622 [0.457, 0.794]	-0.169 [-0.438, 0.107]	0.919 [0.863, 0.957]	0.948 [0.822, 1.054]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.588, 1.073]	0.613 [0.419, 0.832]	0.221 [-0.065, 0.515]	0.919 [0.839, 0.964]	0.999 [0.914, 1.088]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.607, 1.104]	0.621 [0.425, 0.847]	0.132 [-0.159, 0.449]	0.904 [0.822, 0.955]	0.961 [0.861, 1.078]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.508, 1.164]	0.588 [0.385, 0.824]	0.100 [-0.202, 0.403]	0.899 [0.772, 0.970]	0.917 [0.837, 0.979]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.560, 1.250]	0.615 [0.410, 0.864]	-0.025 [-0.350, 0.272]	0.892 [0.754, 0.965]	0.936 [0.851, 1.003]
nb016	MoKa	0.952 [0.702, 1.181]	0.767 [0.565, 0.987]	-0.225 [-0.569, 0.116]	0.895 [0.826, 0.947]	0.935 [0.821, 1.070]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.562, 1.333]	0.640 [0.413, 0.919]	0.003 [-0.317, 0.357]	0.900 [0.760, 0.973]	1.056 [0.956, 1.130]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.692, 1.268]	0.720 [0.501, 0.966]	-0.318 [-0.653, -0.005]	0.915 [0.855, 0.957]	1.089 [0.946, 1.226]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.443, 1.546]	0.561 [0.319, 0.903]	0.103 [-0.212, 0.510]	0.906 [0.826, 0.977]	1.089 [0.958, 1.257]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.465, 1.549]	0.574 [0.330, 0.917]	0.067 [-0.253, 0.466]	0.906 [0.825, 0.976]	1.096 [0.960, 1.261]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.753, 1.253]	0.782 [0.559, 1.015]	0.349 [0.022, 0.687]	0.906 [0.815, 0.956]	1.071 [0.959, 1.183]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.510, 1.541]	0.620 [0.379, 0.952]	0.188 [-0.129, 0.570]	0.878 [0.795, 0.964]	0.997 [0.849, 1.190]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.498, 1.555]	0.608 [0.366, 0.937]	0.083 [-0.242, 0.472]	0.896 [0.822, 0.972]	1.084 [0.966, 1.253]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.501, 1.552]	0.613 [0.362, 0.950]	0.168 [-0.151, 0.571]	0.883 [0.807, 0.967]	1.019 [0.870, 1.214]
arcko	Vertical scheme for type I submission	1.041 [0.732, 1.327]	0.767 [0.532, 1.026]	0.366 [0.032, 0.727]	0.886 [0.803, 0.943]	1.010 [0.900, 1.139]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.708, 1.338]	0.737 [0.498, 1.009]	-0.307 [-0.663, 0.043]	0.913 [0.847, 0.956]	1.125 [1.022, 1.257]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.799, 1.396]	0.841 [0.590, 1.112]	0.277 [-0.102, 0.667]	0.886 [0.775, 0.949]	1.094 [0.981, 1.220]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.611, 1.660]	0.696 [0.417, 1.049]	0.128 [-0.255, 0.554]	0.884 [0.812, 0.961]	1.103 [0.975, 1.290]
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 [0.491, 1.592]
wexjs	Direct scheme for type I submission	1.303 [0.951, 1.633]	0.978 [0.688, 1.303]	0.274 [-0.179, 0.734]	0.859 [0.738, 0.931]	1.134 [0.992, 1.289]
v8qph	ACD/pKa GALAS	1.373 [0.912, 1.787]	0.975 [0.650, 1.347]	-0.145 [-0.637, 0.337]	0.838 [0.700, 0.927]	1.147 [0.967, 1.326]
w4z0e	Direct scheme with single point correction for...	1.569 [1.178, 1.940]	1.226 [0.899, 1.593]	0.090 [-0.471, 0.633]	0.848 [0.761, 0.910]	1.246 [1.084, 1.458]
6tvf8	OE Gaussian Process	1.883 [0.871, 2.851]	1.023 [0.543, 1.646]	0.452 [-0.133, 1.163]	0.515 [0.151, 0.872]	0.584 [0.257, 0.892]
0wfzo	Explicit solvent submission 1	2.894 [1.733, 3.935]	1.880 [1.172, 2.718]	0.762 [-0.159, 1.787]	0.479 [0.209, 0.758]	0.995 [0.585, 1.383]
t8ewk	COSMOlogic_FINE17	3.300 [1.867, 4.401]	1.978 [1.070, 3.016]	1.317 [0.262, 2.507]	0.066 [0.000, 0.457]	0.253 [-0.168, 0.796]
z3btx	Explicit solvent submission 2	4.002 [2.291, 5.431]	2.486 [1.469, 3.670]	1.478 [0.243, 2.855]	0.287 [0.039, 0.607]	0.873 [0.299, 1.437]
758j8	Explicit solvent submission 3	4.524 [2.643, 6.179]	2.949 [1.841, 4.266]	1.846 [0.495, 3.401]	0.242 [0.014, 0.582]	0.864 [0.184, 1.516]
hgn83	Explicit solvent submission 4	6.375 [4.004, 8.442]	4.106 [2.495, 5.887]	2.131 [0.077, 4.317]	0.079 [0.000, 0.406]	0.647 [-0.190, 1.436]

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.