ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.303, 0.642]	0.329 [0.224, 0.453]	-0.019 [-0.190, 0.146]	0.971 [0.935, 0.990]	1.010 [0.966, 1.060]
hdiyq	S+pKa	0.624 [0.471, 0.755]	0.468 [0.326, 0.616]	0.127 [-0.089, 0.343]	0.950 [0.919, 0.975]	0.990 [0.916, 1.086]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.436, 0.811]	0.469 [0.324, 0.632]	-0.024 [-0.247, 0.208]	0.949 [0.889, 0.980]	0.982 [0.913, 1.044]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.465, 0.815]	0.499 [0.357, 0.653]	-0.099 [-0.330, 0.133]	0.948 [0.891, 0.978]	0.995 [0.925, 1.055]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.399, 0.893]	0.434 [0.270, 0.620]	0.113 [-0.114, 0.353]	0.941 [0.874, 0.981]	0.945 [0.867, 1.023]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.441, 0.859]	0.465 [0.311, 0.642]	0.003 [-0.228, 0.238]	0.940 [0.885, 0.977]	0.967 [0.872, 1.049]
nb008	Epik Microscopic	0.761 [0.488, 1.018]	0.523 [0.342, 0.738]	-0.084 [-0.367, 0.173]	0.930 [0.845, 0.976]	0.853 [0.786, 0.925]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.621, 0.941]	0.622 [0.456, 0.800]	-0.169 [-0.438, 0.108]	0.919 [0.864, 0.956]	0.948 [0.820, 1.056]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.583, 1.068]	0.613 [0.419, 0.824]	0.221 [-0.061, 0.514]	0.919 [0.838, 0.964]	0.999 [0.915, 1.085]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.604, 1.096]	0.621 [0.423, 0.844]	0.132 [-0.161, 0.434]	0.904 [0.826, 0.955]	0.961 [0.861, 1.078]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.508, 1.156]	0.588 [0.385, 0.816]	0.100 [-0.205, 0.402]	0.899 [0.776, 0.970]	0.917 [0.838, 0.979]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.555, 1.253]	0.615 [0.408, 0.867]	-0.025 [-0.355, 0.277]	0.892 [0.752, 0.965]	0.936 [0.850, 1.001]
nb016	MoKa	0.952 [0.712, 1.179]	0.767 [0.571, 0.986]	-0.225 [-0.571, 0.120]	0.895 [0.827, 0.946]	0.935 [0.820, 1.071]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.562, 1.325]	0.640 [0.416, 0.908]	0.003 [-0.323, 0.357]	0.900 [0.761, 0.973]	1.056 [0.959, 1.129]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.691, 1.264]	0.720 [0.503, 0.965]	-0.318 [-0.656, -0.008]	0.915 [0.858, 0.956]	1.089 [0.948, 1.220]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.448, 1.549]	0.561 [0.320, 0.906]	0.103 [-0.212, 0.493]	0.906 [0.828, 0.977]	1.089 [0.957, 1.256]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.469, 1.547]	0.574 [0.330, 0.910]	0.067 [-0.257, 0.459]	0.906 [0.828, 0.976]	1.096 [0.960, 1.262]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.752, 1.256]	0.782 [0.557, 1.020]	0.349 [0.023, 0.692]	0.906 [0.815, 0.957]	1.071 [0.965, 1.187]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.511, 1.539]	0.620 [0.380, 0.949]	0.188 [-0.125, 0.575]	0.878 [0.796, 0.964]	0.997 [0.847, 1.189]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.501, 1.542]	0.608 [0.370, 0.933]	0.083 [-0.240, 0.470]	0.896 [0.823, 0.971]	1.084 [0.968, 1.252]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.509, 1.549]	0.613 [0.366, 0.937]	0.168 [-0.157, 0.567]	0.883 [0.808, 0.966]	1.019 [0.869, 1.218]
arcko	Vertical scheme for type I submission	1.041 [0.740, 1.328]	0.767 [0.534, 1.029]	0.366 [0.037, 0.725]	0.886 [0.800, 0.941]	1.010 [0.901, 1.139]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.706, 1.331]	0.737 [0.492, 1.006]	-0.307 [-0.655, 0.039]	0.913 [0.848, 0.956]	1.125 [1.022, 1.257]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.802, 1.397]	0.841 [0.590, 1.115]	0.277 [-0.106, 0.669]	0.886 [0.775, 0.949]	1.094 [0.979, 1.223]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.595, 1.658]	0.696 [0.412, 1.048]	0.128 [-0.255, 0.553]	0.884 [0.808, 0.961]	1.103 [0.974, 1.288]
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 [0.454, 1.000]	1.162 [0.491, 1.592]
wexjs	Direct scheme for type I submission	1.303 [0.942, 1.619]	0.978 [0.675, 1.291]	0.274 [-0.178, 0.738]	0.859 [0.738, 0.929]	1.134 [0.995, 1.290]
v8qph	ACD/pKa GALAS	1.373 [0.910, 1.787]	0.975 [0.650, 1.348]	-0.145 [-0.646, 0.346]	0.838 [0.705, 0.927]	1.147 [0.970, 1.326]
w4z0e	Direct scheme with single point correction for...	1.569 [1.175, 1.938]	1.226 [0.899, 1.586]	0.090 [-0.475, 0.640]	0.848 [0.762, 0.910]	1.246 [1.084, 1.458]
6tvf8	OE Gaussian Process	1.883 [0.875, 2.885]	1.023 [0.542, 1.681]	0.452 [-0.133, 1.198]	0.515 [0.149, 0.874]	0.584 [0.257, 0.891]
0wfzo	Explicit solvent submission 1	2.894 [1.716, 3.931]	1.880 [1.165, 2.717]	0.762 [-0.158, 1.835]	0.479 [0.212, 0.756]	0.995 [0.593, 1.393]
t8ewk	COSMOlogic_FINE17	3.300 [1.888, 4.390]	1.978 [1.074, 3.017]	1.317 [0.272, 2.507]	0.066 [0.000, 0.450]	0.253 [-0.167, 0.784]
z3btx	Explicit solvent submission 2	4.002 [2.327, 5.436]	2.486 [1.478, 3.652]	1.478 [0.279, 2.859]	0.287 [0.036, 0.607]	0.873 [0.289, 1.429]
758j8	Explicit solvent submission 3	4.524 [2.615, 6.103]	2.949 [1.843, 4.191]	1.846 [0.468, 3.299]	0.242 [0.016, 0.578]	0.864 [0.200, 1.505]
hgn83	Explicit solvent submission 4	6.375 [4.062, 8.460]	4.106 [2.521, 5.959]	2.131 [0.085, 4.327]	0.079 [0.000, 0.398]	0.647 [-0.199, 1.426]

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.