ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.390 [0.206, 0.547]	0.317 [0.186, 0.479]	0.153 [-0.075, 0.386]	0.944 [0.151, 0.992]	0.899 [0.252, 0.993]
6tvf8	OE Gaussian Process	0.418 [0.279, 0.552]	0.369 [0.264, 0.505]	-0.105 [-0.359, 0.147]	0.926 [0.333, 0.984]	0.911 [0.565, 1.087]
nb008	Epik Microscopic	0.496 [0.227, 0.707]	0.386 [0.192, 0.610]	-0.052 [-0.382, 0.241]	0.907 [0.072, 0.991]	0.821 [0.021, 1.004]
nb016	MoKa	0.516 [0.253, 0.710]	0.429 [0.234, 0.650]	-0.091 [-0.424, 0.327]	0.922 [0.076, 0.995]	0.991 [0.176, 1.159]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.585 [0.360, 0.845]	0.489 [0.307, 0.735]	0.005 [-0.335, 0.427]	0.867 [0.019, 0.980]	1.009 [-0.175, 1.199]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.609 [0.347, 0.824]	0.474 [0.253, 0.739]	0.006 [-0.356, 0.411]	0.848 [0.097, 0.973]	0.968 [0.484, 1.356]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	0.627 [0.367, 0.846]	0.513 [0.302, 0.743]	0.151 [-0.250, 0.502]	0.839 [0.266, 0.973]	0.763 [0.394, 1.442]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.633 [0.321, 0.946]	0.482 [0.269, 0.783]	0.154 [-0.192, 0.587]	0.833 [0.047, 0.982]	0.777 [0.122, 1.163]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	0.634 [0.325, 0.915]	0.493 [0.264, 0.750]	0.131 [-0.214, 0.529]	0.828 [0.067, 0.983]	0.778 [0.348, 1.113]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.641 [0.268, 0.935]	0.465 [0.216, 0.753]	0.105 [-0.305, 0.482]	0.869 [0.113, 0.979]	0.659 [0.315, 1.030]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	0.647 [0.396, 0.868]	0.540 [0.327, 0.768]	0.204 [-0.186, 0.603]	0.836 [0.269, 0.973]	0.760 [0.393, 1.306]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.649 [0.353, 0.932]	0.493 [0.266, 0.775]	0.137 [-0.236, 0.563]	0.823 [0.054, 0.967]	0.891 [0.306, 1.280]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.662 [0.406, 0.890]	0.549 [0.328, 0.803]	0.053 [-0.313, 0.472]	0.849 [0.058, 0.969]	1.049 [0.321, 1.452]
hdiyq	S+pKa	0.670 [0.463, 0.839]	0.561 [0.329, 0.804]	0.381 [0.041, 0.711]	0.862 [0.339, 0.984]	0.864 [0.423, 1.208]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.679 [0.342, 0.955]	0.537 [0.298, 0.824]	-0.075 [-0.470, 0.345]	0.798 [0.024, 0.971]	0.859 [0.192, 1.145]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.688 [0.297, 1.002]	0.489 [0.211, 0.826]	0.107 [-0.320, 0.578]	0.797 [0.082, 0.967]	0.870 [0.317, 1.331]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	0.699 [0.439, 0.959]	0.594 [0.397, 0.834]	0.084 [-0.339, 0.517]	0.824 [0.165, 0.961]	1.011 [0.559, 1.802]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.700 [0.336, 0.992]	0.513 [0.249, 0.826]	0.187 [-0.272, 0.633]	0.817 [0.080, 0.979]	0.867 [0.251, 1.202]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	0.739 [0.331, 1.119]	0.540 [0.283, 0.893]	0.184 [-0.200, 0.650]	0.828 [0.065, 0.982]	1.052 [0.391, 1.647]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.806 [0.556, 1.029]	0.693 [0.432, 0.946]	0.001 [-0.488, 0.592]	0.705 [0.022, 0.936]	0.722 [-0.320, 1.133]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.848 [0.458, 1.133]	0.651 [0.319, 1.008]	-0.393 [-0.848, 0.058]	0.762 [0.035, 0.941]	0.882 [0.097, 1.073]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.874 [0.549, 1.132]	0.709 [0.404, 1.031]	-0.535 [-0.966, -0.100]	0.796 [0.056, 0.951]	0.900 [0.125, 1.157]
ko8yx	Adiabatic scheme with single point correction ...	0.902 [0.534, 1.279]	0.729 [0.419, 1.111]	0.377 [-0.130, 0.942]	0.790 [0.449, 0.961]	1.065 [0.656, 2.592]
arcko	Vertical scheme for type I submission	0.928 [0.652, 1.182]	0.809 [0.524, 1.100]	0.153 [-0.371, 0.723]	0.683 [0.394, 0.933]	0.892 [0.630, 3.031]
v8qph	ACD/pKa GALAS	0.950 [0.375, 1.510]	0.628 [0.254, 1.161]	-0.076 [-0.705, 0.412]	0.671 [0.054, 0.983]	0.899 [-1.234, 1.153]
wcvnu	Adiabatic scheme for type I submission	1.045 [0.617, 1.450]	0.869 [0.510, 1.281]	0.702 [0.198, 1.248]	0.916 [0.336, 0.989]	1.480 [1.090, 2.427]
y4wws	microscopic pKa prediction with Gaussian and g...	1.081 [0.569, 1.544]	0.836 [0.413, 1.300]	-0.462 [-1.089, 0.142]	0.877 [0.060, 0.986]	1.398 [0.386, 1.912]
wexjs	Direct scheme for type I submission	1.083 [0.654, 1.470]	0.841 [0.431, 1.268]	0.649 [0.107, 1.202]	0.867 [0.562, 0.975]	1.292 [0.849, 2.411]
t8ewk	COSMOlogic_FINE17	1.142 [0.540, 1.684]	0.849 [0.386, 1.380]	-0.381 [-1.059, 0.294]	0.498 [0.000, 0.895]	0.612 [-0.439, 1.088]
qsicn	microscopic pKa prediction with Gaussian and s...	1.261 [0.540, 1.700]	1.120 [0.540, 1.700]	-1.120 [-1.700, -0.540]	1.000 [0.000, 1.000]	1.274 [1.274, nan]
w4z0e	Direct scheme with single point correction for...	1.582 [1.003, 2.094]	1.390 [0.942, 1.892]	0.060 [-0.948, 1.058]	0.720 [0.175, 0.946]	1.504 [0.633, 2.832]
0wfzo	Explicit solvent submission 1	3.720 [1.695, 5.463]	2.680 [1.217, 4.408]	1.146 [-0.991, 3.495]	0.620 [0.138, 0.972]	2.434 [0.600, 5.669]
z3btx	Explicit solvent submission 2	4.319 [2.078, 6.263]	3.231 [1.598, 5.153]	0.941 [-1.447, 3.868]	0.675 [0.022, 0.932]	2.962 [-1.049, 4.450]
758j8	Explicit solvent submission 3	4.605 [1.943, 6.882]	3.461 [1.754, 5.646]	2.103 [-0.409, 4.963]	0.673 [0.025, 0.913]	2.888 [-0.038, 4.326]
hgn83	Explicit solvent submission 4	6.012 [2.934, 8.443]	4.479 [2.166, 6.951]	1.437 [-2.560, 4.886]	0.255 [0.003, 0.865]	2.192 [-0.634, 5.861]

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.