ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.390 [0.218, 0.553]	0.317 [0.193, 0.482]	0.153 [-0.051, 0.376]	0.944 [0.201, 0.990]	0.899 [0.284, 0.988]
6tvf8	OE Gaussian Process	0.418 [0.275, 0.549]	0.369 [0.256, 0.502]	-0.105 [-0.357, 0.146]	0.926 [0.292, 0.986]	0.911 [0.496, 1.094]
nb008	Epik Microscopic	0.496 [0.233, 0.708]	0.386 [0.200, 0.606]	-0.052 [-0.376, 0.256]	0.907 [0.072, 0.991]	0.821 [0.094, 1.014]
nb016	MoKa	0.516 [0.265, 0.715]	0.429 [0.240, 0.661]	-0.091 [-0.461, 0.316]	0.922 [0.027, 0.994]	0.991 [0.051, 1.154]
v8qph	ACD/pKa GALAS	0.530 [0.318, 0.704]	0.414 [0.213, 0.644]	0.199 [-0.153, 0.516]	0.908 [0.029, 0.990]	1.000 [-0.280, 1.146]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.585 [0.350, 0.829]	0.489 [0.311, 0.725]	0.005 [-0.337, 0.404]	0.867 [0.014, 0.981]	1.009 [-0.183, 1.204]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.609 [0.335, 0.814]	0.474 [0.236, 0.725]	0.006 [-0.379, 0.387]	0.848 [0.099, 0.976]	0.968 [0.495, 1.292]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	0.627 [0.354, 0.846]	0.513 [0.293, 0.740]	0.151 [-0.243, 0.526]	0.839 [0.274, 0.969]	0.763 [0.422, 1.282]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.633 [0.315, 0.936]	0.482 [0.257, 0.754]	0.154 [-0.209, 0.576]	0.833 [0.100, 0.982]	0.777 [0.348, 1.118]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	0.634 [0.333, 0.937]	0.493 [0.276, 0.797]	0.131 [-0.207, 0.547]	0.828 [0.064, 0.983]	0.778 [0.285, 1.169]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.641 [0.286, 0.938]	0.465 [0.233, 0.755]	0.105 [-0.295, 0.497]	0.869 [0.159, 0.980]	0.659 [0.365, 1.163]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	0.647 [0.414, 0.862]	0.540 [0.338, 0.753]	0.204 [-0.185, 0.597]	0.836 [0.197, 0.969]	0.760 [0.383, 1.377]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.649 [0.353, 0.944]	0.493 [0.277, 0.783]	0.137 [-0.236, 0.566]	0.823 [0.060, 0.971]	0.891 [0.392, 1.330]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.662 [0.391, 0.892]	0.549 [0.324, 0.804]	0.053 [-0.354, 0.491]	0.849 [0.091, 0.976]	1.049 [0.457, 1.515]
hdiyq	S+pKa	0.670 [0.482, 0.827]	0.561 [0.346, 0.783]	0.381 [0.037, 0.691]	0.862 [0.375, 0.982]	0.864 [0.427, 1.197]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.679 [0.332, 0.955]	0.537 [0.288, 0.833]	-0.075 [-0.461, 0.343]	0.798 [0.056, 0.974]	0.859 [0.086, 1.153]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.688 [0.339, 0.998]	0.489 [0.214, 0.785]	0.107 [-0.282, 0.553]	0.797 [0.122, 0.971]	0.870 [0.340, 1.479]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	0.699 [0.440, 0.955]	0.594 [0.403, 0.832]	0.084 [-0.341, 0.517]	0.824 [0.131, 0.964]	1.011 [0.532, 1.882]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.700 [0.303, 1.014]	0.513 [0.233, 0.831]	0.187 [-0.228, 0.666]	0.817 [0.084, 0.984]	0.867 [0.261, 1.206]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	0.739 [0.314, 1.131]	0.540 [0.272, 0.918]	0.184 [-0.236, 0.659]	0.828 [0.058, 0.985]	1.052 [0.264, 1.596]
t8ewk	COSMOlogic_FINE17	0.793 [0.486, 1.048]	0.638 [0.349, 0.971]	-0.118 [-0.599, 0.422]	0.662 [0.001, 0.931]	0.926 [-1.312, 1.151]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.806 [0.573, 1.023]	0.693 [0.460, 0.966]	0.001 [-0.464, 0.528]	0.705 [0.015, 0.919]	0.722 [-0.513, 1.132]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.848 [0.482, 1.156]	0.651 [0.333, 0.998]	-0.393 [-0.871, 0.038]	0.762 [0.060, 0.956]	0.882 [0.152, 1.073]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.874 [0.555, 1.135]	0.709 [0.402, 1.053]	-0.535 [-0.967, -0.098]	0.796 [0.066, 0.945]	0.900 [0.207, 1.164]
ko8yx	Adiabatic scheme with single point correction ...	0.902 [0.505, 1.287]	0.729 [0.413, 1.135]	0.377 [-0.092, 0.920]	0.790 [0.437, 0.969]	1.065 [0.642, 2.591]
arcko	Vertical scheme for type I submission	0.928 [0.624, 1.210]	0.809 [0.531, 1.114]	0.153 [-0.371, 0.745]	0.683 [0.354, 0.943]	0.892 [0.589, 3.058]
wcvnu	Adiabatic scheme for type I submission	1.045 [0.629, 1.452]	0.869 [0.526, 1.300]	0.702 [0.200, 1.260]	0.916 [0.376, 0.989]	1.480 [1.183, 2.421]
y4wws	microscopic pKa prediction with Gaussian and g...	1.081 [0.608, 1.569]	0.836 [0.450, 1.317]	-0.462 [-1.114, 0.129]	0.877 [0.109, 0.986]	1.398 [0.508, 1.690]
wexjs	Direct scheme for type I submission	1.083 [0.643, 1.482]	0.841 [0.446, 1.300]	0.649 [0.101, 1.220]	0.867 [0.580, 0.975]	1.292 [0.852, 2.396]
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 [1.039, 2.119]	1.390 [0.965, 1.936]	0.060 [-0.915, 1.058]	0.720 [0.229, 0.952]	1.504 [0.617, 2.856]
hgn83	Explicit solvent submission 4	6.012 [2.759, 8.454]	4.479 [2.015, 7.112]	1.437 [-2.168, 4.551]	0.255 [0.001, 0.870]	2.192 [-0.021, 5.654]
758j8	Explicit solvent submission 3	6.120 [2.005, 9.974]	3.890 [1.737, 7.196]	-0.982 [-5.119, 2.148]	0.189 [0.002, 0.937]	1.913 [-2.890, 3.768]
z3btx	Explicit solvent submission 2	7.677 [1.765, 11.571]	4.632 [1.363, 8.484]	-0.048 [-5.487, 4.166]	0.102 [0.001, 0.789]	1.728 [-1.383, 9.459]
0wfzo	Explicit solvent submission 1	8.238 [1.687, 13.717]	4.425 [1.195, 9.550]	-2.029 [-7.830, 2.104]	0.065 [0.001, 0.769]	1.410 [-2.418, 4.832]

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.