ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.509 [0.328, 0.688]	0.377 [0.255, 0.508]	-0.012 [-0.204, 0.166]	0.961 [0.909, 0.987]	1.020 [0.959, 1.095]
hdiyq	S+pKa	0.627 [0.473, 0.771]	0.478 [0.335, 0.640]	0.152 [-0.063, 0.404]	0.948 [0.912, 0.975]	1.038 [0.950, 1.168]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.425, 0.844]	0.495 [0.330, 0.673]	0.026 [-0.223, 0.291]	0.936 [0.853, 0.978]	0.978 [0.910, 1.058]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.465, 0.840]	0.520 [0.377, 0.690]	-0.089 [-0.333, 0.180]	0.943 [0.864, 0.981]	1.039 [0.963, 1.092]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.446, 0.914]	0.495 [0.325, 0.689]	0.058 [-0.186, 0.330]	0.924 [0.850, 0.974]	0.961 [0.841, 1.070]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.421, 0.963]	0.480 [0.296, 0.706]	0.159 [-0.098, 0.440]	0.920 [0.823, 0.974]	0.939 [0.825, 1.056]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.794 [0.491, 1.108]	0.577 [0.388, 0.834]	0.018 [-0.291, 0.340]	0.900 [0.736, 0.971]	0.899 [0.815, 0.967]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.615, 0.963]	0.639 [0.456, 0.825]	-0.243 [-0.510, 0.079]	0.911 [0.810, 0.958]	0.981 [0.815, 1.094]
nb008	Epik Microscopic	0.815 [0.515, 1.105]	0.571 [0.362, 0.820]	-0.080 [-0.404, 0.223]	0.905 [0.790, 0.971]	0.820 [0.742, 0.930]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.847 [0.554, 1.161]	0.631 [0.430, 0.883]	-0.091 [-0.457, 0.243]	0.923 [0.812, 0.976]	1.105 [1.020, 1.194]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.642, 1.169]	0.698 [0.481, 0.932]	0.276 [-0.058, 0.618]	0.892 [0.787, 0.957]	0.997 [0.875, 1.132]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.674, 1.185]	0.711 [0.509, 0.968]	0.172 [-0.193, 0.541]	0.870 [0.750, 0.940]	0.950 [0.817, 1.114]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.578, 1.370]	0.694 [0.450, 0.965]	-0.003 [-0.433, 0.355]	0.853 [0.646, 0.957]	0.920 [0.800, 1.013]
nb016	MoKa	1.010 [0.729, 1.267]	0.815 [0.560, 1.081]	-0.272 [-0.712, 0.148]	0.872 [0.772, 0.939]	0.960 [0.804, 1.157]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.736, 1.361]	0.766 [0.509, 1.045]	-0.409 [-0.769, -0.059]	0.915 [0.829, 0.965]	1.160 [0.978, 1.297]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.467, 1.681]	0.611 [0.330, 0.999]	0.126 [-0.231, 0.605]	0.892 [0.793, 0.975]	1.144 [0.972, 1.366]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.473, 1.727]	0.629 [0.320, 1.033]	0.085 [-0.294, 0.563]	0.892 [0.806, 0.975]	1.152 [0.962, 1.384]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.507, 1.700]	0.665 [0.385, 1.039]	0.238 [-0.133, 0.769]	0.851 [0.764, 0.957]	1.020 [0.822, 1.311]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.514, 1.677]	0.659 [0.376, 1.058]	0.225 [-0.153, 0.673]	0.858 [0.780, 0.958]	1.050 [0.841, 1.308]
arcko	Vertical scheme for type I submission	1.095 [0.763, 1.402]	0.815 [0.552, 1.108]	0.434 [0.066, 0.825]	0.865 [0.763, 0.936]	1.024 [0.892, 1.195]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.818, 1.355]	0.893 [0.643, 1.143]	0.440 [0.040, 0.830]	0.890 [0.762, 0.959]	1.112 [0.967, 1.257]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.499, 1.726]	0.675 [0.375, 1.087]	0.095 [-0.282, 0.601]	0.872 [0.784, 0.967]	1.118 [0.950, 1.365]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.767, 1.460]	0.863 [0.593, 1.170]	-0.367 [-0.787, 0.057]	0.895 [0.783, 0.951]	1.168 [1.028, 1.342]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.320, 1.647]	0.884 [0.234, 1.540]	-0.764 [-1.540, -0.036]	0.914 [0.457, 1.000]	1.162 [0.491, 1.592]
wcvnu	Adiabatic scheme for type I submission	1.190 [0.852, 1.490]	0.960 [0.685, 1.245]	0.331 [-0.112, 0.799]	0.862 [0.695, 0.941]	1.115 [0.962, 1.272]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.652, 1.807]	0.794 [0.466, 1.215]	0.132 [-0.325, 0.648]	0.861 [0.776, 0.952]	1.152 [0.980, 1.406]
6tvf8	OE Gaussian Process	1.326 [0.733, 1.804]	0.853 [0.485, 1.316]	0.156 [-0.373, 0.747]	0.598 [0.275, 0.868]	0.675 [0.410, 0.952]
v8qph	ACD/pKa GALAS	1.424 [0.860, 1.954]	1.019 [0.636, 1.497]	-0.065 [-0.658, 0.522]	0.841 [0.657, 0.940]	1.249 [0.982, 1.487]
wexjs	Direct scheme for type I submission	1.426 [1.055, 1.773]	1.154 [0.836, 1.500]	0.315 [-0.191, 0.890]	0.828 [0.657, 0.923]	1.187 [1.004, 1.409]
w4z0e	Direct scheme with single point correction for...	1.699 [1.286, 2.117]	1.390 [1.042, 1.813]	0.175 [-0.501, 0.785]	0.843 [0.725, 0.914]	1.353 [1.145, 1.651]
0wfzo	Explicit solvent submission 1	2.418 [1.276, 3.492]	1.610 [0.972, 2.322]	0.243 [-0.631, 1.230]	0.527 [0.272, 0.818]	1.080 [0.816, 1.463]
t8ewk	COSMOlogic_FINE17	2.799 [0.944, 4.115]	1.548 [0.721, 2.673]	0.865 [-0.162, 2.109]	0.097 [0.000, 0.822]	0.360 [-0.289, 1.037]
758j8	Explicit solvent submission 3	2.966 [1.879, 4.050]	2.204 [1.514, 3.053]	0.924 [-0.100, 2.096]	0.381 [0.104, 0.656]	0.942 [0.495, 1.423]
z3btx	Explicit solvent submission 2	3.506 [1.557, 5.535]	2.012 [1.089, 3.340]	1.357 [0.239, 2.794]	0.341 [0.170, 0.723]	0.993 [0.751, 1.383]
hgn83	Explicit solvent submission 4	4.519 [2.391, 6.416]	2.875 [1.582, 4.477]	1.417 [-0.240, 3.239]	0.214 [0.040, 0.554]	1.085 [0.564, 1.569]

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.