ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.509 [0.333, 0.701]	0.377 [0.260, 0.523]	-0.012 [-0.215, 0.175]	0.961 [0.907, 0.986]	1.020 [0.958, 1.091]
hdiyq	S+pKa	0.627 [0.462, 0.771]	0.478 [0.327, 0.636]	0.152 [-0.084, 0.382]	0.948 [0.908, 0.975]	1.038 [0.951, 1.159]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.428, 0.851]	0.495 [0.335, 0.675]	0.026 [-0.229, 0.291]	0.936 [0.847, 0.978]	0.978 [0.902, 1.055]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.458, 0.839]	0.520 [0.374, 0.685]	-0.089 [-0.343, 0.165]	0.943 [0.858, 0.981]	1.039 [0.969, 1.092]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.443, 0.907]	0.495 [0.325, 0.692]	0.058 [-0.200, 0.331]	0.924 [0.846, 0.973]	0.961 [0.845, 1.066]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.433, 0.970]	0.480 [0.298, 0.701]	0.159 [-0.104, 0.442]	0.920 [0.822, 0.974]	0.939 [0.834, 1.058]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.794 [0.482, 1.089]	0.577 [0.385, 0.813]	0.018 [-0.302, 0.324]	0.900 [0.750, 0.971]	0.899 [0.822, 0.970]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.620, 0.953]	0.639 [0.460, 0.820]	-0.243 [-0.530, 0.047]	0.911 [0.819, 0.957]	0.981 [0.823, 1.090]
nb008	Epik Microscopic	0.815 [0.506, 1.095]	0.571 [0.362, 0.815]	-0.080 [-0.409, 0.223]	0.905 [0.779, 0.972]	0.820 [0.743, 0.912]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.847 [0.546, 1.153]	0.631 [0.425, 0.874]	-0.091 [-0.424, 0.229]	0.923 [0.812, 0.976]	1.105 [1.019, 1.187]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.643, 1.164]	0.698 [0.483, 0.939]	0.276 [-0.062, 0.622]	0.892 [0.775, 0.955]	0.997 [0.878, 1.121]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.663, 1.180]	0.711 [0.490, 0.947]	0.172 [-0.178, 0.521]	0.870 [0.753, 0.939]	0.950 [0.818, 1.117]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.596, 1.354]	0.694 [0.461, 0.980]	-0.003 [-0.393, 0.348]	0.853 [0.657, 0.954]	0.920 [0.800, 1.007]
nb016	MoKa	1.010 [0.736, 1.258]	0.815 [0.579, 1.066]	-0.272 [-0.670, 0.123]	0.872 [0.776, 0.936]	0.960 [0.802, 1.147]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.716, 1.358]	0.766 [0.504, 1.052]	-0.409 [-0.788, -0.051]	0.915 [0.826, 0.963]	1.160 [0.993, 1.297]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.463, 1.672]	0.611 [0.327, 1.008]	0.126 [-0.246, 0.592]	0.892 [0.801, 0.975]	1.144 [0.969, 1.356]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.482, 1.676]	0.629 [0.340, 1.021]	0.085 [-0.288, 0.552]	0.892 [0.799, 0.974]	1.152 [0.972, 1.359]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.520, 1.666]	0.665 [0.392, 1.051]	0.238 [-0.126, 0.682]	0.851 [0.770, 0.956]	1.020 [0.820, 1.290]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.517, 1.682]	0.659 [0.374, 1.052]	0.225 [-0.150, 0.682]	0.858 [0.783, 0.958]	1.050 [0.846, 1.327]
arcko	Vertical scheme for type I submission	1.095 [0.741, 1.407]	0.815 [0.546, 1.112]	0.434 [0.057, 0.823]	0.865 [0.757, 0.934]	1.024 [0.894, 1.204]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.834, 1.354]	0.893 [0.658, 1.146]	0.440 [0.056, 0.816]	0.890 [0.761, 0.957]	1.112 [0.967, 1.252]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.523, 1.673]	0.675 [0.392, 1.052]	0.095 [-0.292, 0.551]	0.872 [0.790, 0.964]	1.118 [0.955, 1.353]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.784, 1.456]	0.863 [0.598, 1.163]	-0.367 [-0.792, 0.041]	0.895 [0.806, 0.949]	1.168 [1.027, 1.345]
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]
wcvnu	Adiabatic scheme for type I submission	1.190 [0.876, 1.494]	0.960 [0.703, 1.242]	0.331 [-0.100, 0.770]	0.862 [0.697, 0.941]	1.115 [0.957, 1.276]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.656, 1.798]	0.794 [0.464, 1.194]	0.132 [-0.320, 0.649]	0.861 [0.778, 0.951]	1.152 [0.980, 1.415]
6tvf8	OE Gaussian Process	1.326 [0.738, 1.792]	0.853 [0.479, 1.277]	0.156 [-0.349, 0.701]	0.598 [0.263, 0.867]	0.675 [0.395, 0.947]
v8qph	ACD/pKa GALAS	1.424 [0.895, 1.882]	1.019 [0.639, 1.434]	-0.065 [-0.653, 0.502]	0.841 [0.665, 0.941]	1.249 [1.000, 1.463]
wexjs	Direct scheme for type I submission	1.426 [1.070, 1.757]	1.154 [0.845, 1.490]	0.315 [-0.212, 0.886]	0.828 [0.648, 0.926]	1.187 [0.985, 1.401]
w4z0e	Direct scheme with single point correction for...	1.699 [1.280, 2.090]	1.390 [1.028, 1.787]	0.175 [-0.477, 0.819]	0.843 [0.725, 0.916]	1.353 [1.136, 1.638]
0wfzo	Explicit solvent submission 1	2.418 [1.314, 3.543]	1.610 [1.001, 2.393]	0.243 [-0.627, 1.236]	0.527 [0.281, 0.797]	1.080 [0.810, 1.460]
t8ewk	COSMOlogic_FINE17	2.799 [0.933, 4.049]	1.548 [0.706, 2.605]	0.865 [-0.110, 2.059]	0.097 [0.000, 0.807]	0.360 [-0.315, 1.030]
758j8	Explicit solvent submission 3	2.966 [1.890, 4.040]	2.204 [1.516, 3.047]	0.924 [-0.129, 2.065]	0.381 [0.124, 0.650]	0.942 [0.515, 1.419]
z3btx	Explicit solvent submission 2	3.506 [1.508, 5.338]	2.012 [1.049, 3.271]	1.357 [0.247, 2.764]	0.341 [0.150, 0.727]	0.993 [0.727, 1.418]
hgn83	Explicit solvent submission 4	4.519 [2.377, 6.400]	2.875 [1.580, 4.471]	1.417 [-0.211, 3.308]	0.214 [0.038, 0.540]	1.085 [0.573, 1.566]

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.