ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.509 [0.335, 0.688]	0.377 [0.258, 0.508]	-0.012 [-0.232, 0.188]	0.961 [0.903, 0.986]	1.020 [0.956, 1.089]
hdiyq	S+pKa	0.627 [0.460, 0.786]	0.478 [0.326, 0.646]	0.152 [-0.087, 0.387]	0.948 [0.913, 0.976]	1.038 [0.947, 1.160]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.428, 0.838]	0.495 [0.329, 0.669]	0.026 [-0.236, 0.270]	0.936 [0.852, 0.978]	0.978 [0.907, 1.050]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.452, 0.835]	0.520 [0.373, 0.680]	-0.089 [-0.367, 0.166]	0.943 [0.851, 0.981]	1.039 [0.961, 1.090]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.439, 0.912]	0.495 [0.320, 0.698]	0.058 [-0.228, 0.318]	0.924 [0.852, 0.973]	0.961 [0.844, 1.067]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.416, 0.997]	0.480 [0.277, 0.729]	0.159 [-0.128, 0.446]	0.920 [0.806, 0.974]	0.939 [0.829, 1.066]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.626, 0.961]	0.639 [0.459, 0.834]	-0.243 [-0.558, 0.074]	0.911 [0.820, 0.959]	0.981 [0.821, 1.093]
nb008	Epik Microscopic	0.815 [0.507, 1.126]	0.571 [0.365, 0.825]	-0.080 [-0.409, 0.233]	0.905 [0.774, 0.973]	0.820 [0.747, 0.911]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.639, 1.169]	0.698 [0.471, 0.949]	0.276 [-0.080, 0.630]	0.892 [0.769, 0.958]	0.997 [0.881, 1.119]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.932 [0.556, 1.279]	0.655 [0.421, 0.942]	0.118 [-0.215, 0.476]	0.861 [0.670, 0.960]	0.878 [0.763, 0.953]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.662, 1.200]	0.711 [0.482, 0.980]	0.172 [-0.159, 0.578]	0.870 [0.745, 0.938]	0.950 [0.813, 1.124]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.586, 1.381]	0.694 [0.449, 0.987]	-0.003 [-0.401, 0.367]	0.853 [0.648, 0.958]	0.920 [0.800, 1.013]
nb016	MoKa	1.010 [0.746, 1.261]	0.815 [0.569, 1.062]	-0.272 [-0.667, 0.134]	0.872 [0.770, 0.937]	0.960 [0.808, 1.167]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	1.041 [0.589, 1.459]	0.730 [0.448, 1.054]	0.036 [-0.367, 0.470]	0.871 [0.650, 0.972]	1.075 [0.913, 1.168]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.731, 1.357]	0.766 [0.511, 1.057]	-0.409 [-0.771, -0.057]	0.915 [0.824, 0.964]	1.160 [0.993, 1.299]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.461, 1.661]	0.611 [0.317, 0.992]	0.126 [-0.259, 0.552]	0.892 [0.805, 0.977]	1.144 [0.965, 1.337]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.490, 1.659]	0.629 [0.343, 1.016]	0.085 [-0.288, 0.576]	0.892 [0.794, 0.974]	1.152 [0.968, 1.369]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.526, 1.665]	0.665 [0.393, 1.062]	0.238 [-0.142, 0.683]	0.851 [0.763, 0.958]	1.020 [0.821, 1.300]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.526, 1.670]	0.659 [0.376, 1.025]	0.225 [-0.161, 0.679]	0.858 [0.780, 0.958]	1.050 [0.836, 1.316]
arcko	Vertical scheme for type I submission	1.095 [0.746, 1.426]	0.815 [0.565, 1.119]	0.434 [0.052, 0.830]	0.865 [0.764, 0.936]	1.024 [0.893, 1.218]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.827, 1.361]	0.893 [0.651, 1.150]	0.440 [0.036, 0.822]	0.890 [0.745, 0.961]	1.112 [0.952, 1.250]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.537, 1.701]	0.675 [0.393, 1.048]	0.095 [-0.299, 0.563]	0.872 [0.788, 0.966]	1.118 [0.955, 1.352]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.794, 1.440]	0.863 [0.593, 1.162]	-0.367 [-0.758, 0.060]	0.895 [0.789, 0.953]	1.168 [1.029, 1.349]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.320, 1.647]	0.884 [0.270, 1.540]	-0.764 [-1.540, 0.012]	0.914 [0.457, 1.000]	1.162 [0.640, 1.579]
wcvnu	Adiabatic scheme for type I submission	1.190 [0.881, 1.509]	0.960 [0.709, 1.241]	0.331 [-0.093, 0.781]	0.862 [0.685, 0.943]	1.115 [0.943, 1.284]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.658, 1.820]	0.794 [0.474, 1.209]	0.132 [-0.323, 0.669]	0.861 [0.777, 0.949]	1.152 [0.963, 1.422]
wexjs	Direct scheme for type I submission	1.426 [1.091, 1.788]	1.154 [0.863, 1.523]	0.315 [-0.196, 0.906]	0.828 [0.633, 0.922]	1.187 [0.987, 1.421]
v8qph	ACD/pKa GALAS	1.486 [1.002, 1.922]	1.080 [0.706, 1.498]	-0.164 [-0.753, 0.416]	0.813 [0.621, 0.928]	1.226 [0.968, 1.426]
w4z0e	Direct scheme with single point correction for...	1.699 [1.264, 2.096]	1.390 [1.030, 1.780]	0.175 [-0.483, 0.828]	0.843 [0.719, 0.917]	1.353 [1.138, 1.625]
6tvf8	OE Gaussian Process	2.031 [0.966, 3.103]	1.131 [0.570, 1.910]	0.462 [-0.284, 1.315]	0.324 [0.024, 0.816]	0.432 [0.086, 0.873]
0wfzo	Explicit solvent submission 1	2.968 [1.615, 4.067]	1.957 [1.199, 2.871]	0.642 [-0.365, 1.906]	0.355 [0.081, 0.708]	0.862 [0.385, 1.388]
t8ewk	COSMOlogic_FINE17	3.128 [1.515, 4.273]	1.801 [0.795, 2.864]	1.260 [0.114, 2.386]	0.092 [0.001, 0.622]	0.313 [-0.134, 0.970]
z3btx	Explicit solvent submission 2	3.692 [1.777, 5.468]	2.243 [1.257, 3.642]	1.049 [-0.196, 2.623]	0.178 [0.002, 0.654]	0.643 [-0.032, 1.309]
758j8	Explicit solvent submission 3	4.214 [2.023, 6.079]	2.743 [1.620, 4.138]	1.512 [0.109, 3.158]	0.123 [0.000, 0.599]	0.572 [-0.262, 1.327]
hgn83	Explicit solvent submission 4	6.196 [3.448, 8.660]	3.985 [2.218, 6.046]	2.711 [0.681, 5.068]	0.022 [0.000, 0.351]	0.321 [-0.588, 1.303]

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.