ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.509 [0.331, 0.695]	0.377 [0.257, 0.519]	-0.012 [-0.216, 0.177]	0.961 [0.907, 0.987]	1.020 [0.958, 1.091]
hdiyq	S+pKa	0.627 [0.461, 0.769]	0.478 [0.327, 0.638]	0.152 [-0.080, 0.387]	0.948 [0.911, 0.975]	1.038 [0.949, 1.160]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.652 [0.427, 0.844]	0.495 [0.338, 0.670]	0.026 [-0.235, 0.294]	0.936 [0.852, 0.978]	0.978 [0.901, 1.052]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.655 [0.462, 0.842]	0.520 [0.375, 0.686]	-0.089 [-0.342, 0.172]	0.943 [0.858, 0.980]	1.039 [0.968, 1.092]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.691 [0.441, 0.903]	0.495 [0.320, 0.687]	0.058 [-0.198, 0.334]	0.924 [0.846, 0.973]	0.961 [0.848, 1.064]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.703 [0.424, 0.963]	0.480 [0.293, 0.700]	0.159 [-0.098, 0.438]	0.920 [0.820, 0.974]	0.939 [0.834, 1.054]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.798 [0.617, 0.957]	0.639 [0.458, 0.825]	-0.243 [-0.530, 0.056]	0.911 [0.815, 0.958]	0.981 [0.826, 1.090]
nb008	Epik Microscopic	0.815 [0.507, 1.102]	0.571 [0.362, 0.814]	-0.080 [-0.414, 0.228]	0.905 [0.780, 0.972]	0.820 [0.744, 0.912]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.912 [0.633, 1.163]	0.698 [0.473, 0.939]	0.276 [-0.057, 0.616]	0.892 [0.780, 0.956]	0.997 [0.877, 1.117]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.932 [0.554, 1.264]	0.655 [0.427, 0.929]	0.118 [-0.232, 0.469]	0.861 [0.667, 0.960]	0.878 [0.764, 0.955]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.933 [0.659, 1.183]	0.711 [0.486, 0.951]	0.172 [-0.174, 0.522]	0.870 [0.757, 0.938]	0.950 [0.820, 1.116]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.965 [0.599, 1.352]	0.694 [0.465, 0.972]	-0.003 [-0.391, 0.350]	0.853 [0.653, 0.954]	0.920 [0.798, 1.011]
nb016	MoKa	1.010 [0.731, 1.259]	0.815 [0.577, 1.068]	-0.272 [-0.668, 0.126]	0.872 [0.777, 0.936]	0.960 [0.803, 1.152]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	1.041 [0.615, 1.440]	0.730 [0.475, 1.042]	0.036 [-0.351, 0.453]	0.871 [0.668, 0.967]	1.075 [0.922, 1.170]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.043 [0.722, 1.360]	0.766 [0.508, 1.051]	-0.409 [-0.783, -0.033]	0.915 [0.823, 0.963]	1.160 [0.992, 1.296]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	1.073 [0.459, 1.674]	0.611 [0.328, 1.012]	0.126 [-0.237, 0.600]	0.892 [0.804, 0.975]	1.144 [0.966, 1.355]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.085 [0.482, 1.681]	0.629 [0.342, 1.027]	0.085 [-0.285, 0.560]	0.892 [0.801, 0.973]	1.152 [0.971, 1.368]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.086 [0.521, 1.654]	0.665 [0.397, 1.037]	0.238 [-0.137, 0.689]	0.851 [0.768, 0.956]	1.020 [0.817, 1.289]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.095 [0.512, 1.686]	0.659 [0.376, 1.058]	0.225 [-0.151, 0.695]	0.858 [0.780, 0.959]	1.050 [0.845, 1.325]
arcko	Vertical scheme for type I submission	1.095 [0.749, 1.410]	0.815 [0.548, 1.117]	0.434 [0.058, 0.831]	0.865 [0.759, 0.933]	1.024 [0.897, 1.201]
ko8yx	Adiabatic scheme with single point correction ...	1.098 [0.828, 1.354]	0.893 [0.655, 1.149]	0.440 [0.050, 0.823]	0.890 [0.758, 0.957]	1.112 [0.963, 1.255]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.105 [0.522, 1.686]	0.675 [0.396, 1.057]	0.095 [-0.285, 0.578]	0.872 [0.792, 0.964]	1.118 [0.956, 1.358]
y4wws	microscopic pKa prediction with Gaussian and g...	1.137 [0.790, 1.448]	0.863 [0.596, 1.162]	-0.367 [-0.777, 0.052]	0.895 [0.801, 0.949]	1.168 [1.029, 1.348]
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 [0.454, 1.000]	1.162 [0.491, 1.579]
wcvnu	Adiabatic scheme for type I submission	1.190 [0.875, 1.493]	0.960 [0.701, 1.240]	0.331 [-0.104, 0.764]	0.862 [0.706, 0.943]	1.115 [0.964, 1.276]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.237 [0.660, 1.816]	0.794 [0.465, 1.214]	0.132 [-0.316, 0.644]	0.861 [0.778, 0.951]	1.152 [0.977, 1.424]
wexjs	Direct scheme for type I submission	1.426 [1.066, 1.760]	1.154 [0.838, 1.486]	0.315 [-0.214, 0.873]	0.828 [0.648, 0.925]	1.187 [0.988, 1.406]
v8qph	ACD/pKa GALAS	1.486 [0.984, 1.933]	1.080 [0.698, 1.516]	-0.164 [-0.752, 0.413]	0.813 [0.615, 0.926]	1.226 [0.979, 1.436]
w4z0e	Direct scheme with single point correction for...	1.699 [1.277, 2.073]	1.390 [1.025, 1.765]	0.175 [-0.483, 0.811]	0.843 [0.729, 0.914]	1.353 [1.134, 1.632]
6tvf8	OE Gaussian Process	2.031 [0.890, 3.063]	1.131 [0.560, 1.856]	0.462 [-0.228, 1.308]	0.324 [0.023, 0.807]	0.432 [0.089, 0.876]
0wfzo	Explicit solvent submission 1	2.968 [1.631, 4.121]	1.957 [1.174, 2.895]	0.642 [-0.382, 1.813]	0.355 [0.076, 0.712]	0.862 [0.349, 1.374]
t8ewk	COSMOlogic_FINE17	3.128 [1.617, 4.334]	1.801 [0.851, 2.918]	1.260 [0.198, 2.507]	0.092 [0.000, 0.591]	0.313 [-0.168, 0.974]
z3btx	Explicit solvent submission 2	3.692 [1.753, 5.323]	2.243 [1.240, 3.478]	1.049 [-0.228, 2.508]	0.178 [0.002, 0.664]	0.643 [-0.034, 1.276]
758j8	Explicit solvent submission 3	4.214 [2.071, 6.024]	2.743 [1.658, 4.061]	1.512 [0.102, 3.098]	0.123 [0.001, 0.589]	0.572 [-0.222, 1.316]
hgn83	Explicit solvent submission 4	6.196 [3.448, 8.542]	3.985 [2.316, 5.978]	2.711 [0.699, 5.022]	0.022 [0.000, 0.338]	0.321 [-0.598, 1.280]

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.