ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.307, 0.660]	0.329 [0.224, 0.462]	-0.019 [-0.176, 0.143]	0.971 [0.937, 0.989]	1.010 [0.966, 1.063]
hdiyq	S+pKa	0.624 [0.481, 0.760]	0.468 [0.327, 0.619]	0.127 [-0.090, 0.325]	0.950 [0.918, 0.974]	0.990 [0.919, 1.097]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.427, 0.807]	0.469 [0.320, 0.638]	-0.024 [-0.247, 0.202]	0.949 [0.892, 0.981]	0.982 [0.911, 1.046]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.470, 0.827]	0.499 [0.360, 0.664]	-0.099 [-0.316, 0.156]	0.948 [0.887, 0.978]	0.995 [0.921, 1.058]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.398, 0.888]	0.434 [0.271, 0.618]	0.113 [-0.122, 0.365]	0.941 [0.877, 0.980]	0.945 [0.866, 1.023]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.433, 0.838]	0.465 [0.300, 0.629]	0.003 [-0.237, 0.263]	0.940 [0.887, 0.978]	0.967 [0.870, 1.049]
nb008	Epik Microscopic	0.761 [0.474, 1.012]	0.523 [0.339, 0.720]	-0.084 [-0.339, 0.179]	0.930 [0.843, 0.978]	0.853 [0.788, 0.924]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.618, 0.938]	0.622 [0.448, 0.794]	-0.169 [-0.438, 0.116]	0.919 [0.870, 0.960]	0.948 [0.822, 1.059]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.583, 1.075]	0.613 [0.415, 0.832]	0.221 [-0.078, 0.513]	0.919 [0.835, 0.967]	0.999 [0.915, 1.087]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.603, 1.112]	0.621 [0.428, 0.847]	0.132 [-0.151, 0.441]	0.904 [0.830, 0.956]	0.961 [0.868, 1.099]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.518, 1.160]	0.588 [0.395, 0.827]	0.100 [-0.196, 0.419]	0.899 [0.778, 0.970]	0.917 [0.840, 0.980]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.557, 1.256]	0.615 [0.413, 0.877]	-0.025 [-0.346, 0.292]	0.892 [0.758, 0.966]	0.936 [0.847, 1.008]
nb016	MoKa	0.952 [0.701, 1.170]	0.767 [0.569, 0.977]	-0.225 [-0.564, 0.133]	0.895 [0.825, 0.949]	0.935 [0.818, 1.070]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.578, 1.356]	0.640 [0.420, 0.957]	0.003 [-0.322, 0.376]	0.900 [0.752, 0.974]	1.056 [0.950, 1.130]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.686, 1.274]	0.720 [0.498, 0.968]	-0.318 [-0.656, -0.003]	0.915 [0.855, 0.958]	1.089 [0.943, 1.227]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.454, 1.525]	0.561 [0.317, 0.868]	0.103 [-0.205, 0.500]	0.906 [0.826, 0.977]	1.089 [0.964, 1.262]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.454, 1.553]	0.574 [0.329, 0.917]	0.067 [-0.247, 0.458]	0.906 [0.828, 0.976]	1.096 [0.968, 1.253]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.731, 1.290]	0.782 [0.548, 1.030]	0.349 [0.018, 0.703]	0.906 [0.819, 0.957]	1.071 [0.951, 1.193]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.502, 1.549]	0.620 [0.385, 0.939]	0.188 [-0.122, 0.594]	0.878 [0.800, 0.965]	0.997 [0.843, 1.205]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.512, 1.627]	0.608 [0.366, 0.960]	0.083 [-0.240, 0.497]	0.896 [0.821, 0.972]	1.084 [0.969, 1.269]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.516, 1.565]	0.613 [0.379, 0.931]	0.168 [-0.146, 0.592]	0.883 [0.810, 0.965]	1.019 [0.870, 1.243]
arcko	Vertical scheme for type I submission	1.041 [0.743, 1.330]	0.767 [0.532, 1.038]	0.366 [0.031, 0.721]	0.886 [0.802, 0.943]	1.010 [0.897, 1.140]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.724, 1.340]	0.737 [0.514, 1.010]	-0.307 [-0.665, 0.041]	0.913 [0.847, 0.955]	1.125 [1.021, 1.273]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.794, 1.387]	0.841 [0.599, 1.107]	0.277 [-0.081, 0.670]	0.886 [0.777, 0.950]	1.094 [0.987, 1.217]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.613, 1.668]	0.696 [0.411, 1.085]	0.128 [-0.239, 0.588]	0.884 [0.812, 0.962]	1.103 [0.977, 1.327]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.320, 1.643]	0.884 [0.234, 1.540]	-0.764 [-1.540, 0.030]	0.914 [0.457, 1.000]	1.162 [0.491, 1.579]
wexjs	Direct scheme for type I submission	1.303 [0.957, 1.637]	0.978 [0.680, 1.290]	0.274 [-0.190, 0.762]	0.859 [0.741, 0.932]	1.134 [0.988, 1.305]
v8qph	ACD/pKa GALAS	1.373 [0.902, 1.808]	0.975 [0.653, 1.343]	-0.145 [-0.635, 0.362]	0.838 [0.697, 0.924]	1.147 [0.972, 1.331]
w4z0e	Direct scheme with single point correction for...	1.569 [1.152, 1.934]	1.226 [0.869, 1.581]	0.090 [-0.484, 0.665]	0.848 [0.758, 0.913]	1.246 [1.080, 1.457]
6tvf8	OE Gaussian Process	1.883 [0.875, 2.851]	1.023 [0.555, 1.707]	0.452 [-0.159, 1.174]	0.515 [0.144, 0.887]	0.584 [0.252, 0.897]
0wfzo	Explicit solvent submission 1	2.894 [1.661, 4.037]	1.880 [1.134, 2.861]	0.762 [-0.171, 1.953]	0.479 [0.187, 0.763]	0.995 [0.587, 1.386]
t8ewk	COSMOlogic_FINE17	3.300 [1.853, 4.353]	1.978 [1.038, 2.959]	1.317 [0.275, 2.434]	0.066 [0.000, 0.451]	0.253 [-0.137, 0.788]
z3btx	Explicit solvent submission 2	4.002 [2.186, 5.477]	2.486 [1.425, 3.727]	1.478 [0.186, 2.836]	0.287 [0.045, 0.626]	0.873 [0.313, 1.451]
758j8	Explicit solvent submission 3	4.524 [2.607, 6.358]	2.949 [1.858, 4.373]	1.846 [0.435, 3.523]	0.242 [0.018, 0.586]	0.864 [0.220, 1.488]
hgn83	Explicit solvent submission 4	6.375 [4.075, 8.572]	4.106 [2.514, 5.988]	2.131 [0.143, 4.484]	0.079 [0.000, 0.403]	0.647 [-0.220, 1.452]

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.