ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.302, 0.642]	0.329 [0.224, 0.455]	-0.019 [-0.191, 0.137]	0.971 [0.935, 0.989]	1.010 [0.965, 1.060]
hdiyq	S+pKa	0.607 [0.453, 0.741]	0.450 [0.309, 0.596]	0.098 [-0.122, 0.309]	0.950 [0.913, 0.975]	1.011 [0.931, 1.111]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.436, 0.811]	0.469 [0.325, 0.636]	-0.024 [-0.244, 0.211]	0.949 [0.888, 0.980]	0.982 [0.914, 1.046]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.465, 0.814]	0.499 [0.359, 0.651]	-0.099 [-0.324, 0.125]	0.948 [0.891, 0.978]	0.995 [0.924, 1.055]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.663 [0.413, 0.908]	0.443 [0.281, 0.637]	0.111 [-0.115, 0.354]	0.938 [0.863, 0.978]	0.943 [0.856, 1.028]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.439, 0.858]	0.465 [0.309, 0.643]	0.003 [-0.222, 0.245]	0.940 [0.886, 0.977]	0.967 [0.867, 1.051]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.723 [0.425, 1.003]	0.504 [0.336, 0.708]	-0.017 [-0.288, 0.237]	0.925 [0.816, 0.979]	0.949 [0.890, 1.002]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.760 [0.586, 0.908]	0.596 [0.429, 0.766]	-0.221 [-0.475, 0.040]	0.924 [0.855, 0.962]	0.982 [0.859, 1.076]
nb008	Epik Microscopic	0.761 [0.481, 1.023]	0.523 [0.340, 0.735]	-0.084 [-0.367, 0.168]	0.930 [0.848, 0.976]	0.853 [0.785, 0.926]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.781 [0.505, 1.057]	0.555 [0.372, 0.766]	-0.104 [-0.387, 0.174]	0.940 [0.865, 0.980]	1.077 [1.014, 1.142]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.590, 1.088]	0.633 [0.432, 0.849]	0.230 [-0.077, 0.531]	0.914 [0.826, 0.963]	0.994 [0.906, 1.087]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.595, 1.093]	0.621 [0.419, 0.839]	0.132 [-0.158, 0.431]	0.904 [0.823, 0.956]	0.961 [0.861, 1.078]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.553, 1.248]	0.615 [0.408, 0.864]	-0.025 [-0.355, 0.272]	0.892 [0.757, 0.966]	0.936 [0.852, 1.001]
nb016	MoKa	0.952 [0.709, 1.180]	0.767 [0.566, 0.982]	-0.225 [-0.572, 0.107]	0.895 [0.826, 0.946]	0.935 [0.821, 1.067]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.690, 1.264]	0.720 [0.500, 0.961]	-0.318 [-0.653, 0.003]	0.915 [0.859, 0.957]	1.089 [0.950, 1.222]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.449, 1.535]	0.561 [0.317, 0.900]	0.103 [-0.215, 0.491]	0.906 [0.828, 0.976]	1.089 [0.960, 1.254]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.462, 1.540]	0.574 [0.326, 0.908]	0.067 [-0.258, 0.454]	0.906 [0.828, 0.976]	1.096 [0.961, 1.256]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.755, 1.251]	0.782 [0.562, 1.009]	0.349 [0.022, 0.689]	0.906 [0.813, 0.955]	1.071 [0.963, 1.182]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.512, 1.540]	0.620 [0.381, 0.942]	0.188 [-0.132, 0.569]	0.878 [0.797, 0.964]	0.997 [0.846, 1.190]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.497, 1.545]	0.608 [0.366, 0.935]	0.083 [-0.243, 0.471]	0.896 [0.821, 0.972]	1.084 [0.967, 1.252]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.510, 1.553]	0.613 [0.371, 0.945]	0.168 [-0.150, 0.566]	0.883 [0.805, 0.965]	1.019 [0.867, 1.219]
arcko	Vertical scheme for type I submission	1.041 [0.745, 1.328]	0.767 [0.533, 1.035]	0.366 [0.037, 0.719]	0.886 [0.800, 0.942]	1.010 [0.901, 1.141]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.701, 1.350]	0.737 [0.489, 1.019]	-0.307 [-0.676, 0.032]	0.913 [0.848, 0.956]	1.125 [1.023, 1.261]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.797, 1.399]	0.841 [0.591, 1.110]	0.277 [-0.095, 0.672]	0.886 [0.773, 0.949]	1.094 [0.982, 1.224]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.598, 1.642]	0.696 [0.410, 1.044]	0.128 [-0.255, 0.553]	0.884 [0.813, 0.961]	1.103 [0.976, 1.285]
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]
6tvf8	OE Gaussian Process	1.251 [0.733, 1.679]	0.789 [0.462, 1.169]	0.199 [-0.251, 0.662]	0.736 [0.482, 0.910]	0.762 [0.549, 0.934]
v8qph	ACD/pKa GALAS	1.314 [0.833, 1.747]	0.921 [0.602, 1.298]	-0.062 [-0.555, 0.417]	0.859 [0.740, 0.940]	1.163 [0.987, 1.344]
wexjs	Direct scheme for type I submission	1.325 [0.979, 1.652]	1.009 [0.715, 1.331]	0.281 [-0.174, 0.772]	0.847 [0.703, 0.926]	1.146 [0.993, 1.312]
w4z0e	Direct scheme with single point correction for...	1.569 [1.160, 1.951]	1.226 [0.890, 1.592]	0.090 [-0.483, 0.633]	0.848 [0.765, 0.910]	1.246 [1.081, 1.453]
t8ewk	COSMOlogic_FINE17	2.685 [0.876, 3.885]	1.437 [0.648, 2.421]	0.808 [-0.088, 1.912]	0.130 [0.000, 0.835]	0.408 [-0.217, 1.042]
758j8	Explicit solvent submission 3	4.301 [2.137, 6.454]	2.650 [1.626, 4.029]	0.339 [-1.292, 1.716]	0.258 [0.076, 0.665]	0.972 [0.650, 1.353]
z3btx	Explicit solvent submission 2	4.825 [1.885, 7.327]	2.528 [1.282, 4.162]	0.554 [-1.284, 2.192]	0.247 [0.076, 0.724]	1.057 [0.751, 1.391]
0wfzo	Explicit solvent submission 1	4.972 [1.379, 8.168]	2.237 [1.010, 4.136]	-0.638 [-2.700, 0.864]	0.196 [0.049, 0.786]	0.990 [0.711, 1.300]
hgn83	Explicit solvent submission 4	5.111 [3.167, 6.835]	3.207 [1.875, 4.786]	1.006 [-0.840, 2.882]	0.271 [0.096, 0.560]	1.254 [0.865, 1.705]

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.