ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.307, 0.651]	0.329 [0.225, 0.474]	-0.019 [-0.194, 0.134]	0.971 [0.933, 0.989]	1.010 [0.967, 1.058]
hdiyq	S+pKa	0.607 [0.458, 0.748]	0.450 [0.315, 0.606]	0.098 [-0.118, 0.314]	0.950 [0.916, 0.975]	1.011 [0.933, 1.118]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.439, 0.807]	0.469 [0.320, 0.630]	-0.024 [-0.235, 0.209]	0.949 [0.890, 0.979]	0.982 [0.904, 1.048]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.480, 0.821]	0.499 [0.366, 0.666]	-0.099 [-0.335, 0.132]	0.948 [0.887, 0.978]	0.995 [0.923, 1.053]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.663 [0.409, 0.908]	0.443 [0.283, 0.641]	0.111 [-0.132, 0.346]	0.938 [0.865, 0.979]	0.943 [0.857, 1.031]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.451, 0.844]	0.465 [0.316, 0.634]	0.003 [-0.220, 0.237]	0.940 [0.888, 0.975]	0.967 [0.866, 1.051]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.723 [0.413, 1.014]	0.504 [0.334, 0.714]	-0.017 [-0.311, 0.255]	0.925 [0.818, 0.979]	0.949 [0.888, 1.002]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.760 [0.608, 0.906]	0.596 [0.445, 0.761]	-0.221 [-0.497, 0.044]	0.924 [0.857, 0.961]	0.982 [0.844, 1.078]
nb008	Epik Microscopic	0.761 [0.489, 1.025]	0.523 [0.344, 0.752]	-0.084 [-0.366, 0.156]	0.930 [0.849, 0.976]	0.853 [0.784, 0.929]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.781 [0.503, 1.076]	0.555 [0.368, 0.772]	-0.104 [-0.408, 0.179]	0.940 [0.863, 0.979]	1.077 [1.016, 1.145]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.592, 1.095]	0.633 [0.439, 0.863]	0.230 [-0.067, 0.559]	0.914 [0.834, 0.965]	0.994 [0.908, 1.096]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.625, 1.107]	0.621 [0.431, 0.852]	0.132 [-0.145, 0.463]	0.904 [0.828, 0.953]	0.961 [0.858, 1.077]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.550, 1.249]	0.615 [0.403, 0.874]	-0.025 [-0.330, 0.297]	0.892 [0.736, 0.968]	0.936 [0.844, 1.001]
nb016	MoKa	0.952 [0.726, 1.176]	0.767 [0.569, 0.994]	-0.225 [-0.595, 0.118]	0.895 [0.826, 0.944]	0.935 [0.827, 1.078]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.681, 1.270]	0.720 [0.495, 0.963]	-0.318 [-0.637, 0.011]	0.915 [0.850, 0.957]	1.089 [0.954, 1.217]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.433, 1.558]	0.561 [0.313, 0.922]	0.103 [-0.197, 0.508]	0.906 [0.826, 0.980]	1.089 [0.960, 1.258]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.461, 1.551]	0.574 [0.321, 0.908]	0.067 [-0.253, 0.441]	0.906 [0.827, 0.978]	1.096 [0.967, 1.256]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.761, 1.281]	0.782 [0.570, 1.039]	0.349 [0.002, 0.710]	0.906 [0.822, 0.956]	1.071 [0.968, 1.194]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.503, 1.605]	0.620 [0.379, 0.975]	0.188 [-0.129, 0.591]	0.878 [0.801, 0.964]	0.997 [0.848, 1.196]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.493, 1.594]	0.608 [0.361, 0.938]	0.083 [-0.223, 0.514]	0.896 [0.817, 0.974]	1.084 [0.970, 1.261]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.511, 1.574]	0.613 [0.376, 0.968]	0.168 [-0.149, 0.593]	0.883 [0.806, 0.966]	1.019 [0.875, 1.225]
arcko	Vertical scheme for type I submission	1.041 [0.736, 1.332]	0.767 [0.548, 1.038]	0.366 [0.033, 0.752]	0.886 [0.798, 0.942]	1.010 [0.892, 1.141]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.695, 1.348]	0.737 [0.487, 1.036]	-0.307 [-0.683, 0.026]	0.913 [0.844, 0.959]	1.125 [1.016, 1.264]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.812, 1.397]	0.841 [0.594, 1.106]	0.277 [-0.104, 0.669]	0.886 [0.770, 0.944]	1.094 [0.982, 1.221]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.580, 1.645]	0.696 [0.405, 1.034]	0.128 [-0.250, 0.555]	0.884 [0.803, 0.967]	1.103 [0.979, 1.273]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.296, 1.660]	0.884 [0.228, 1.576]	-0.764 [-1.576, 0.060]	0.914 [0.454, 1.000]	1.162 [0.491, 1.579]
6tvf8	OE Gaussian Process	1.251 [0.725, 1.704]	0.789 [0.466, 1.178]	0.199 [-0.251, 0.707]	0.736 [0.472, 0.914]	0.762 [0.555, 0.927]
v8qph	ACD/pKa GALAS	1.314 [0.824, 1.731]	0.921 [0.616, 1.304]	-0.062 [-0.531, 0.401]	0.859 [0.747, 0.942]	1.163 [0.978, 1.346]
wexjs	Direct scheme for type I submission	1.325 [0.960, 1.651]	1.009 [0.713, 1.331]	0.281 [-0.195, 0.753]	0.847 [0.682, 0.923]	1.146 [0.986, 1.302]
w4z0e	Direct scheme with single point correction for...	1.569 [1.154, 1.938]	1.226 [0.875, 1.604]	0.090 [-0.452, 0.620]	0.848 [0.760, 0.910]	1.246 [1.075, 1.460]
t8ewk	COSMOlogic_FINE17	2.685 [0.876, 3.903]	1.437 [0.620, 2.404]	0.808 [-0.119, 1.932]	0.130 [0.001, 0.859]	0.408 [-0.245, 1.047]
758j8	Explicit solvent submission 3	4.301 [2.104, 6.343]	2.650 [1.616, 4.045]	0.339 [-1.400, 1.749]	0.258 [0.074, 0.678]	0.972 [0.654, 1.339]
z3btx	Explicit solvent submission 2	4.825 [1.820, 7.577]	2.528 [1.219, 4.259]	0.554 [-1.386, 2.210]	0.247 [0.074, 0.744]	1.057 [0.749, 1.382]
0wfzo	Explicit solvent submission 1	4.972 [1.449, 8.287]	2.237 [1.058, 4.206]	-0.638 [-2.669, 0.844]	0.196 [0.050, 0.791]	0.990 [0.672, 1.290]
hgn83	Explicit solvent submission 4	5.111 [3.157, 6.837]	3.207 [1.846, 4.818]	1.006 [-0.816, 2.930]	0.271 [0.082, 0.567]	1.254 [0.844, 1.762]

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.