ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.303, 0.643]	0.329 [0.225, 0.455]	-0.019 [-0.190, 0.140]	0.971 [0.935, 0.990]	1.010 [0.966, 1.062]
hdiyq	S+pKa	0.624 [0.471, 0.759]	0.468 [0.325, 0.619]	0.127 [-0.091, 0.341]	0.950 [0.917, 0.975]	0.990 [0.917, 1.089]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.436, 0.811]	0.469 [0.327, 0.634]	-0.024 [-0.250, 0.211]	0.949 [0.890, 0.980]	0.982 [0.912, 1.043]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.464, 0.817]	0.499 [0.360, 0.653]	-0.099 [-0.322, 0.132]	0.948 [0.889, 0.978]	0.995 [0.924, 1.056]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.401, 0.887]	0.434 [0.271, 0.620]	0.113 [-0.106, 0.346]	0.941 [0.876, 0.980]	0.945 [0.867, 1.021]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.436, 0.856]	0.465 [0.305, 0.635]	0.003 [-0.225, 0.247]	0.940 [0.886, 0.977]	0.967 [0.870, 1.049]
nb008	Epik Microscopic	0.761 [0.482, 1.010]	0.523 [0.340, 0.729]	-0.084 [-0.365, 0.177]	0.930 [0.848, 0.976]	0.853 [0.785, 0.927]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.618, 0.933]	0.622 [0.456, 0.792]	-0.169 [-0.438, 0.109]	0.919 [0.865, 0.958]	0.948 [0.820, 1.052]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.586, 1.069]	0.613 [0.421, 0.827]	0.221 [-0.071, 0.511]	0.919 [0.840, 0.965]	0.999 [0.914, 1.087]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.603, 1.096]	0.621 [0.420, 0.835]	0.132 [-0.163, 0.436]	0.904 [0.824, 0.955]	0.961 [0.859, 1.080]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.506, 1.173]	0.588 [0.385, 0.831]	0.100 [-0.185, 0.396]	0.899 [0.770, 0.970]	0.917 [0.838, 0.978]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.559, 1.246]	0.615 [0.412, 0.863]	-0.025 [-0.353, 0.272]	0.892 [0.758, 0.964]	0.936 [0.851, 1.000]
nb016	MoKa	0.952 [0.708, 1.180]	0.767 [0.565, 0.983]	-0.225 [-0.569, 0.113]	0.895 [0.827, 0.946]	0.935 [0.824, 1.072]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.559, 1.325]	0.640 [0.409, 0.911]	0.003 [-0.331, 0.344]	0.900 [0.760, 0.973]	1.056 [0.957, 1.130]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.686, 1.262]	0.720 [0.497, 0.965]	-0.318 [-0.652, -0.002]	0.915 [0.856, 0.956]	1.089 [0.943, 1.218]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.452, 1.539]	0.561 [0.322, 0.902]	0.103 [-0.206, 0.494]	0.906 [0.825, 0.977]	1.089 [0.957, 1.255]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.466, 1.540]	0.574 [0.329, 0.912]	0.067 [-0.253, 0.455]	0.906 [0.828, 0.976]	1.096 [0.961, 1.259]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.756, 1.254]	0.782 [0.566, 1.020]	0.349 [0.021, 0.684]	0.906 [0.815, 0.955]	1.071 [0.964, 1.184]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.515, 1.538]	0.620 [0.382, 0.934]	0.188 [-0.132, 0.568]	0.878 [0.801, 0.964]	0.997 [0.845, 1.190]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.500, 1.560]	0.613 [0.361, 0.950]	0.168 [-0.154, 0.568]	0.883 [0.807, 0.966]	1.019 [0.866, 1.215]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.505, 1.548]	0.608 [0.371, 0.939]	0.083 [-0.244, 0.470]	0.896 [0.822, 0.970]	1.084 [0.970, 1.257]
arcko	Vertical scheme for type I submission	1.041 [0.736, 1.326]	0.767 [0.533, 1.027]	0.366 [0.033, 0.715]	0.886 [0.803, 0.943]	1.010 [0.902, 1.139]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.711, 1.333]	0.737 [0.495, 1.003]	-0.307 [-0.669, 0.037]	0.913 [0.848, 0.957]	1.125 [1.023, 1.259]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.795, 1.395]	0.841 [0.593, 1.113]	0.277 [-0.102, 0.658]	0.886 [0.775, 0.950]	1.094 [0.978, 1.220]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.602, 1.655]	0.696 [0.413, 1.050]	0.128 [-0.250, 0.552]	0.884 [0.812, 0.962]	1.103 [0.976, 1.289]
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]
wexjs	Direct scheme for type I submission	1.303 [0.956, 1.633]	0.978 [0.683, 1.300]	0.274 [-0.166, 0.734]	0.859 [0.735, 0.929]	1.134 [0.995, 1.291]
v8qph	ACD/pKa GALAS	1.373 [0.906, 1.784]	0.975 [0.651, 1.349]	-0.145 [-0.632, 0.342]	0.838 [0.708, 0.927]	1.147 [0.972, 1.327]
w4z0e	Direct scheme with single point correction for...	1.569 [1.171, 1.945]	1.226 [0.900, 1.595]	0.090 [-0.481, 0.642]	0.848 [0.764, 0.909]	1.246 [1.084, 1.460]
6tvf8	OE Gaussian Process	1.883 [0.866, 2.861]	1.023 [0.537, 1.659]	0.452 [-0.139, 1.163]	0.515 [0.153, 0.873]	0.584 [0.255, 0.890]
0wfzo	Explicit solvent submission 1	2.894 [1.728, 3.910]	1.880 [1.165, 2.689]	0.762 [-0.156, 1.772]	0.479 [0.209, 0.756]	0.995 [0.593, 1.379]
t8ewk	COSMOlogic_FINE17	3.300 [1.884, 4.387]	1.978 [1.071, 3.008]	1.317 [0.260, 2.506]	0.066 [0.000, 0.448]	0.253 [-0.174, 0.777]
z3btx	Explicit solvent submission 2	4.002 [2.274, 5.460]	2.486 [1.469, 3.701]	1.478 [0.239, 2.860]	0.287 [0.043, 0.603]	0.873 [0.308, 1.437]
758j8	Explicit solvent submission 3	4.524 [2.659, 6.162]	2.949 [1.856, 4.271]	1.846 [0.499, 3.383]	0.242 [0.017, 0.577]	0.864 [0.209, 1.514]
hgn83	Explicit solvent submission 4	6.375 [4.056, 8.495]	4.106 [2.496, 5.970]	2.131 [0.050, 4.302]	0.079 [0.000, 0.403]	0.647 [-0.193, 1.450]

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.