ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.305, 0.622]	0.329 [0.224, 0.443]	-0.019 [-0.185, 0.147]	0.971 [0.940, 0.990]	1.010 [0.969, 1.060]
hdiyq	S+pKa	0.624 [0.474, 0.753]	0.468 [0.329, 0.615]	0.127 [-0.085, 0.341]	0.950 [0.920, 0.974]	0.990 [0.919, 1.082]
epvmk	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	0.631 [0.429, 0.812]	0.469 [0.323, 0.641]	-0.024 [-0.261, 0.239]	0.949 [0.894, 0.981]	0.982 [0.912, 1.043]
xnoe0	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	0.647 [0.468, 0.830]	0.499 [0.363, 0.670]	-0.099 [-0.349, 0.132]	0.948 [0.885, 0.979]	0.995 [0.920, 1.055]
gdqeg	PCM/B3LYP/6-311+G(d,p)	0.653 [0.406, 0.886]	0.434 [0.275, 0.616]	0.113 [-0.100, 0.339]	0.941 [0.875, 0.981]	0.945 [0.860, 1.028]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.444, 0.871]	0.465 [0.312, 0.639]	0.003 [-0.220, 0.244]	0.940 [0.887, 0.979]	0.967 [0.878, 1.049]
nb008	Epik Microscopic	0.761 [0.485, 1.035]	0.523 [0.341, 0.753]	-0.084 [-0.404, 0.187]	0.930 [0.844, 0.977]	0.853 [0.780, 0.930]
ccpmw	ReSCoSS conformations // COSMOtherm pKa	0.788 [0.608, 0.937]	0.622 [0.443, 0.798]	-0.169 [-0.430, 0.101]	0.919 [0.863, 0.957]	0.948 [0.826, 1.051]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.584, 1.064]	0.613 [0.421, 0.819]	0.221 [-0.075, 0.509]	0.919 [0.835, 0.965]	0.999 [0.915, 1.091]
cywyk	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	0.860 [0.602, 1.093]	0.621 [0.416, 0.846]	0.132 [-0.172, 0.426]	0.904 [0.825, 0.956]	0.961 [0.866, 1.079]
ftc8w	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	0.861 [0.523, 1.170]	0.588 [0.395, 0.836]	0.100 [-0.199, 0.417]	0.899 [0.770, 0.968]	0.917 [0.839, 0.980]
nxaaw	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	0.894 [0.562, 1.253]	0.615 [0.415, 0.881]	-0.025 [-0.329, 0.277]	0.892 [0.754, 0.965]	0.936 [0.850, 1.009]
nb016	MoKa	0.952 [0.715, 1.170]	0.767 [0.573, 0.975]	-0.225 [-0.565, 0.117]	0.895 [0.828, 0.947]	0.935 [0.825, 1.056]
kxztt	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	0.959 [0.574, 1.343]	0.640 [0.430, 0.925]	0.003 [-0.324, 0.381]	0.900 [0.753, 0.972]	1.056 [0.955, 1.135]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.683, 1.271]	0.720 [0.490, 0.973]	-0.318 [-0.658, 0.012]	0.915 [0.860, 0.957]	1.089 [0.953, 1.227]
cm2yq	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.994 [0.454, 1.550]	0.561 [0.317, 0.915]	0.103 [-0.207, 0.496]	0.906 [0.830, 0.977]	1.089 [0.966, 1.244]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.465, 1.618]	0.574 [0.319, 0.943]	0.067 [-0.280, 0.461]	0.906 [0.815, 0.978]	1.096 [0.967, 1.266]
ko8yx	Adiabatic scheme with single point correction ...	1.012 [0.731, 1.269]	0.782 [0.558, 1.019]	0.349 [0.017, 0.699]	0.906 [0.805, 0.956]	1.071 [0.960, 1.180]
wuuvc	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.016 [0.517, 1.539]	0.620 [0.391, 0.948]	0.188 [-0.130, 0.586]	0.878 [0.793, 0.965]	0.997 [0.857, 1.185]
z7fhp	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	1.022 [0.473, 1.560]	0.608 [0.349, 0.960]	0.083 [-0.260, 0.481]	0.896 [0.828, 0.975]	1.084 [0.966, 1.253]
ktpj5	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.022 [0.506, 1.557]	0.613 [0.368, 0.939]	0.168 [-0.151, 0.604]	0.883 [0.805, 0.965]	1.019 [0.864, 1.220]
arcko	Vertical scheme for type I submission	1.041 [0.736, 1.321]	0.767 [0.525, 1.013]	0.366 [0.053, 0.709]	0.886 [0.815, 0.941]	1.010 [0.897, 1.147]
y4wws	microscopic pKa prediction with Gaussian and g...	1.042 [0.698, 1.351]	0.737 [0.482, 1.019]	-0.307 [-0.686, 0.045]	0.913 [0.845, 0.958]	1.125 [1.025, 1.268]
wcvnu	Adiabatic scheme for type I submission	1.108 [0.827, 1.404]	0.841 [0.608, 1.114]	0.277 [-0.113, 0.674]	0.886 [0.768, 0.948]	1.094 [0.979, 1.220]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.622, 1.679]	0.696 [0.424, 1.073]	0.128 [-0.244, 0.609]	0.884 [0.812, 0.962]	1.103 [0.966, 1.288]
qsicn	microscopic pKa prediction with Gaussian and s...	1.165 [0.296, 1.660]	0.884 [0.228, 1.540]	-0.764 [-1.540, 0.012]	0.914 [0.454, 1.000]	1.162 [0.491, 2.305]
wexjs	Direct scheme for type I submission	1.303 [0.965, 1.639]	0.978 [0.693, 1.334]	0.274 [-0.156, 0.771]	0.859 [0.731, 0.936]	1.134 [0.991, 1.298]
v8qph	ACD/pKa GALAS	1.373 [0.939, 1.805]	0.975 [0.657, 1.345]	-0.145 [-0.633, 0.355]	0.838 [0.701, 0.927]	1.147 [0.983, 1.325]
w4z0e	Direct scheme with single point correction for...	1.569 [1.184, 1.946]	1.226 [0.909, 1.581]	0.090 [-0.519, 0.647]	0.848 [0.766, 0.912]	1.246 [1.097, 1.450]
6tvf8	OE Gaussian Process	1.883 [0.847, 2.799]	1.023 [0.525, 1.609]	0.452 [-0.157, 1.093]	0.515 [0.147, 0.891]	0.584 [0.252, 0.896]
0wfzo	Explicit solvent submission 1	2.894 [1.690, 3.879]	1.880 [1.129, 2.722]	0.762 [-0.205, 1.753]	0.479 [0.198, 0.760]	0.995 [0.570, 1.390]
t8ewk	COSMOlogic_FINE17	3.300 [1.907, 4.475]	1.978 [1.075, 3.102]	1.317 [0.247, 2.584]	0.066 [0.000, 0.457]	0.253 [-0.201, 0.812]
z3btx	Explicit solvent submission 2	4.002 [2.429, 5.482]	2.486 [1.541, 3.727]	1.478 [0.272, 2.954]	0.287 [0.034, 0.612]	0.873 [0.296, 1.472]
758j8	Explicit solvent submission 3	4.524 [2.523, 6.157]	2.949 [1.875, 4.215]	1.846 [0.463, 3.277]	0.242 [0.014, 0.594]	0.864 [0.191, 1.570]
hgn83	Explicit solvent submission 4	6.375 [4.084, 8.346]	4.106 [2.568, 5.798]	2.131 [0.051, 4.349]	0.079 [0.001, 0.418]	0.647 [-0.133, 1.485]

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.