ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.298, 0.647]	0.329 [0.222, 0.457]	-0.019 [-0.190, 0.140]	0.971 [0.934, 0.990]	1.010 [0.966, 1.062]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.440, 0.859]	0.465 [0.310, 0.639]	0.003 [-0.222, 0.240]	0.940 [0.887, 0.977]	0.967 [0.869, 1.049]
nb008	Epik Microscopic	0.761 [0.481, 1.023]	0.523 [0.338, 0.735]	-0.084 [-0.371, 0.170]	0.930 [0.845, 0.976]	0.853 [0.786, 0.925]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.838 [0.585, 1.074]	0.613 [0.422, 0.829]	0.221 [-0.065, 0.516]	0.919 [0.840, 0.965]	0.999 [0.915, 1.086]
nb016	MoKa	0.952 [0.710, 1.179]	0.767 [0.567, 0.984]	-0.225 [-0.575, 0.108]	0.895 [0.826, 0.946]	0.935 [0.820, 1.073]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.691, 1.263]	0.720 [0.498, 0.959]	-0.318 [-0.647, -0.005]	0.915 [0.856, 0.957]	1.089 [0.945, 1.220]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.465, 1.543]	0.574 [0.328, 0.908]	0.067 [-0.253, 0.467]	0.906 [0.829, 0.976]	1.096 [0.961, 1.262]
arcko	Vertical scheme for type I submission	1.041 [0.732, 1.323]	0.767 [0.531, 1.030]	0.366 [0.039, 0.717]	0.886 [0.801, 0.942]	1.010 [0.900, 1.138]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.605, 1.665]	0.696 [0.414, 1.052]	0.128 [-0.258, 0.559]	0.884 [0.812, 0.961]	1.103 [0.976, 1.297]
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 [0.454, 1.000]	1.162 [0.519, 1.592]
6tvf8	OE Gaussian Process	1.883 [0.877, 2.845]	1.023 [0.536, 1.654]	0.452 [-0.138, 1.184]	0.515 [0.158, 0.876]	0.584 [0.262, 0.891]
0wfzo	Explicit solvent submission 1	2.894 [1.734, 3.931]	1.880 [1.170, 2.730]	0.762 [-0.165, 1.832]	0.479 [0.213, 0.751]	0.995 [0.602, 1.391]
758j8	Explicit solvent submission 3	4.524 [2.631, 6.160]	2.949 [1.843, 4.258]	1.846 [0.481, 3.422]	0.242 [0.015, 0.579]	0.864 [0.195, 1.503]

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.