ID	name	RMSE	MAE	ME	R^2	m
nb011	Jaguar	0.468 [0.304, 0.644]	0.329 [0.224, 0.456]	-0.019 [-0.187, 0.143]	0.971 [0.935, 0.990]	1.010 [0.966, 1.061]
4o0ia	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	0.664 [0.440, 0.855]	0.465 [0.309, 0.637]	0.003 [-0.225, 0.247]	0.940 [0.885, 0.977]	0.967 [0.870, 1.050]
nb008	Epik Microscopic	0.761 [0.485, 1.023]	0.523 [0.340, 0.737]	-0.084 [-0.372, 0.168]	0.930 [0.848, 0.976]	0.853 [0.784, 0.926]
0xi4b	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	0.853 [0.602, 1.096]	0.633 [0.437, 0.856]	0.230 [-0.059, 0.538]	0.914 [0.825, 0.963]	0.994 [0.906, 1.089]
nb016	MoKa	0.952 [0.709, 1.172]	0.767 [0.566, 0.977]	-0.225 [-0.564, 0.122]	0.895 [0.827, 0.946]	0.935 [0.821, 1.076]
eyetm	ReSCoSS conformations // DSD-BLYP-D3 reranking...	0.979 [0.693, 1.269]	0.720 [0.499, 0.965]	-0.318 [-0.656, -0.001]	0.915 [0.856, 0.957]	1.089 [0.949, 1.222]
2umai	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	1.004 [0.465, 1.560]	0.574 [0.329, 0.913]	0.067 [-0.252, 0.478]	0.906 [0.828, 0.976]	1.096 [0.963, 1.259]
arcko	Vertical scheme for type I submission	1.041 [0.736, 1.325]	0.767 [0.529, 1.029]	0.366 [0.032, 0.725]	0.886 [0.802, 0.942]	1.010 [0.903, 1.139]
8toyp	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	1.134 [0.602, 1.672]	0.696 [0.413, 1.060]	0.128 [-0.253, 0.560]	0.884 [0.811, 0.961]	1.103 [0.975, 1.294]
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	1.251 [0.735, 1.685]	0.789 [0.461, 1.176]	0.199 [-0.245, 0.674]	0.736 [0.474, 0.910]	0.762 [0.547, 0.931]
758j8	Explicit solvent submission 3	4.301 [2.156, 6.456]	2.650 [1.637, 4.047]	0.339 [-1.319, 1.747]	0.258 [0.074, 0.660]	0.972 [0.638, 1.355]
0wfzo	Explicit solvent submission 1	4.972 [1.387, 8.192]	2.237 [1.013, 4.163]	-0.638 [-2.719, 0.832]	0.196 [0.049, 0.784]	0.990 [0.709, 1.303]

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.