

ID	name	RMSE	MAE	ME	R ²	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.546, 0.811]	0.579 [0.451, 0.712]	0.235 [-0.009, 0.459]	0.937 [0.878, 0.972]	0.923 [0.839, 1.015]
gyuhx	S+pKa	0.732 [0.556, 0.912]	0.585 [0.435, 0.745]	0.035 [-0.232, 0.286]	0.929 [0.877, 0.965]	0.979 [0.904, 1.083]
xmyhm	ACD/pKa Classic	0.787 [0.522, 1.041]	0.564 [0.384, 0.776]	0.134 [-0.141, 0.402]	0.919 [0.847, 0.968]	0.961 [0.858, 1.079]
nb017	MoKa	0.943 [0.721, 1.153]	0.770 [0.584, 0.970]	-0.162 [-0.496, 0.159]	0.884 [0.807, 0.937]	0.939 [0.821, 1.075]
nb007	Epik Scan	0.946 [0.729, 1.159]	0.776 [0.589, 0.973]	0.045 [-0.303, 0.368]	0.879 [0.759, 0.946]	0.840 [0.767, 0.923]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.780, 1.229]	0.799 [0.588, 1.020]	-0.166 [-0.504, 0.203]	0.867 [0.784, 0.933]	0.927 [0.762, 1.081]
nb010	Epik Microscopic	1.028 [0.771, 1.265]	0.814 [0.605, 1.042]	0.243 [-0.115, 0.587]	0.869 [0.772, 0.940]	0.946 [0.827, 1.078]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.781, 1.361]	0.814 [0.578, 1.069]	-0.475 [-0.825, -0.137]	0.906 [0.839, 0.952]	1.078 [0.933, 1.221]
nb013	Jaguar	1.103 [0.711, 1.466]	0.803 [0.557, 1.085]	-0.148 [-0.547, 0.221]	0.884 [0.782, 0.947]	1.092 [0.903, 1.256]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.993, 1.572]	1.044 [0.800, 1.310]	0.129 [-0.319, 0.562]	0.874 [0.802, 0.932]	1.162 [0.942, 1.340]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.428, 1.720]	-0.924 [-1.720, -0.108]	0.910 [0.509, 1.000]	1.185 [0.339, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.929, 1.837]	1.008 [0.678, 1.375]	-0.183 [-0.690, 0.316]	0.834 [0.695, 0.927]	1.155 [0.983, 1.332]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.140, 2.043]	1.239 [0.906, 1.614]	-0.316 [-0.883, 0.219]	0.803 [0.668, 0.904]	1.140 [0.976, 1.341]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.199, 2.064]	1.296 [0.958, 1.656]	-0.122 [-0.713, 0.436]	0.813 [0.689, 0.908]	1.198 [1.027, 1.399]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.067, 2.371]	1.213 [0.852, 1.663]	0.442 [-0.105, 1.042]	0.797 [0.698, 0.898]	1.156 [0.954, 1.433]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.082, 2.389]	1.246 [0.883, 1.697]	0.509 [-0.035, 1.110]	0.796 [0.698, 0.898]	1.153 [0.950, 1.423]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	-1.006 [-2.178, 0.134]	0.919 [0.463, 1.000]	1.446 [0.735, 2.147]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.424, 2.111]	1.500 [1.172, 1.836]	1.298 [0.865, 1.716]	0.910 [0.862, 0.949]	1.229 [1.059, 1.404]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.300, 2.247]	1.389 [1.003, 1.806]	-0.744 [-1.317, -0.154]	0.792 [0.655, 0.895]	1.149 [0.962, 1.373]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.389, 2.221]	1.482 [1.129, 1.865]	0.103 [-0.541, 0.720]	0.820 [0.701, 0.906]	1.294 [1.118, 1.503]
5byn6	Adiabatic scheme for type III submission	1.890 [1.500, 2.269]	1.588 [1.236, 1.965]	1.317 [0.823, 1.804]	0.905 [0.852, 0.948]	1.284 [1.105, 1.469]
y75vj	Direct scheme for type III submission	1.901 [1.493, 2.268]	1.584 [1.215, 1.972]	1.039 [0.467, 1.601]	0.891 [0.791, 0.953]	1.345 [1.159, 1.529]
w4iyd	Vertical scheme for type III submission	1.926 [1.527, 2.286]	1.584 [1.207, 1.984]	1.257 [0.741, 1.775]	0.853 [0.741, 0.922]	1.206 [1.001, 1.403]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.212, 2.732]	1.435 [1.038, 1.951]	-0.467 [-1.067, 0.241]	0.709 [0.602, 0.868]	1.083 [0.802, 1.451]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.383, 2.646]	1.568 [1.167, 2.050]	0.557 [-0.105, 1.256]	0.823 [0.724, 0.903]	1.350 [1.151, 1.600]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.383, 2.649]	1.577 [1.174, 2.054]	0.524 [-0.139, 1.227]	0.825 [0.724, 0.904]	1.358 [1.158, 1.607]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.722, 2.320]	1.805 [1.471, 2.129]	-0.405 [-1.075, 0.319]	0.469 [0.286, 0.641]	0.559 [0.348, 0.829]
hytjn	OE Gaussian Process	2.161 [1.245, 3.091]	1.389 [0.856, 2.052]	0.709 [0.033, 1.512]	0.449 [0.129, 0.781]	0.621 [0.257, 1.001]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.371, 2.960]	1.578 [1.091, 2.158]	-0.733 [-1.415, 0.043]	0.769 [0.665, 0.891]	1.291 [1.014, 1.629]
q3pfp	OE Gaussian Process Resampled	2.193 [1.332, 3.086]	1.505 [0.998, 2.137]	0.589 [-0.118, 1.388]	0.443 [0.126, 0.768]	0.658 [0.268, 1.067]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.617, 2.813]	1.778 [1.342, 2.269]	0.784 [0.086, 1.525]	0.822 [0.690, 0.905]	1.406 [1.201, 1.628]
xikp8	Direct scheme with single point correction for...	2.348 [1.937, 2.722]	2.056 [1.658, 2.461]	0.773 [-0.029, 1.557]	0.890 [0.800, 0.947]	1.588 [1.397, 1.801]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.786, 2.941]	1.915 [1.437, 2.428]	0.313 [-0.510, 1.137]	0.842 [0.741, 0.914]	1.557 [1.344, 1.818]
5nm4j	Substructure matches from experimental data	2.450 [1.410, 3.335]	1.583 [0.941, 2.331]	0.046 [-0.817, 1.037]	0.192 [0.002, 0.699]	0.398 [-0.067, 0.827]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.695, 3.298]	1.826 [1.257, 2.483]	-0.651 [-1.488, 0.236]	0.761 [0.633, 0.873]	1.432 [1.126, 1.783]
pwn3m	Analog_search	2.604 [1.416, 3.522]	1.539 [0.805, 2.369]	0.788 [-0.086, 1.769]	0.208 [0.003, 0.639]	0.369 [0.009, 0.785]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.346, 3.570]	2.525 [1.978, 3.104]	0.424 [-0.611, 1.484]	0.844 [0.739, 0.916]	1.784 [1.550, 2.060]
0hxtm	COSMOtherm_FINE17	3.263 [1.829, 4.398]	1.918 [1.038, 2.979]	1.377 [0.380, 2.562]	0.075 [0.000, 0.472]	0.281 [-0.173, 0.831]

Notes

- Mean and 95% confidence intervals of statistic values were calculated by bootstrapping.
- Submissions with submission IDs nb001, nb002, nb003, nb004, nb005 and nb005 include non-blind corrections to pKa predictions of only SM22 molecule. pKas of the rest of the molecules in these submissions were blindly predicted before experimental data was released.

- 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.