

ID	name	RMSE	MAE	ME	R ²	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.546, 0.811]	0.579 [0.450, 0.710]	-0.235 [-0.461, 0.001]	0.937 [0.878, 0.972]	1.015 [0.913, 1.115]
gyuhx	S+pKa	0.730 [0.552, 0.916]	0.579 [0.429, 0.749]	-0.009 [-0.265, 0.260]	0.925 [0.868, 0.963]	0.929 [0.814, 1.031]
xmyhm	ACD/pKa Classic	0.774 [0.492, 1.034]	0.546 [0.363, 0.761]	-0.102 [-0.370, 0.181]	0.916 [0.829, 0.969]	0.934 [0.818, 1.043]
yqkga	ReSCoSS conformations // COSMOtherm pKa	0.903 [0.685, 1.117]	0.710 [0.518, 0.919]	0.288 [-0.026, 0.579]	0.901 [0.821, 0.953]	0.901 [0.776, 1.041]
nb007	Epik-sequential	0.968 [0.764, 1.175]	0.810 [0.628, 1.005]	-0.025 [-0.357, 0.325]	0.871 [0.762, 0.936]	0.997 [0.858, 1.119]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.780, 1.356]	0.814 [0.579, 1.070]	0.475 [0.139, 0.822]	0.906 [0.840, 0.951]	0.840 [0.747, 0.957]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.718]	1.084 [0.428, 1.704]	0.924 [0.108, 1.704]	0.910 [0.509, 1.000]	0.768 [0.558, 1.516]
37xm8	ACD/pKa GALAS	1.358 [0.844, 1.811]	0.955 [0.632, 1.331]	0.101 [-0.400, 0.601]	0.854 [0.730, 0.939]	0.729 [0.599, 0.877]
hytjn	OE Gaussian Process	1.434 [0.976, 1.832]	1.034 [0.676, 1.422]	-0.240 [-0.778, 0.276]	0.675 [0.420, 0.853]	0.795 [0.601, 1.003]
q3pfp	OE Gaussian Process Resampled	1.484 [1.049, 1.865]	1.140 [0.808, 1.497]	-0.090 [-0.667, 0.445]	0.667 [0.430, 0.837]	0.752 [0.570, 0.968]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.150, 2.037]	1.239 [0.915, 1.612]	0.316 [-0.222, 0.883]	0.803 [0.670, 0.904]	0.705 [0.569, 0.835]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.683 [1.205, 2.131]	1.304 [0.948, 1.695]	1.061 [0.616, 1.535]	0.837 [0.729, 0.916]	0.780 [0.637, 0.925]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.702 [1.063, 2.391]	1.219 [0.842, 1.682]	-0.422 [-1.025, 0.144]	0.792 [0.686, 0.898]	0.664 [0.519, 0.856]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	1.006 [-0.134, 2.178]	0.919 [0.463, 1.000]	0.635 [0.394, 0.806]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.720 [1.080, 2.405]	1.250 [0.875, 1.709]	-0.467 [-1.087, 0.104]	0.794 [0.685, 0.900]	0.662 [0.514, 0.850]
ryzue	Adiabatic scheme with single point correction ...	1.745 [1.370, 2.101]	1.436 [1.094, 1.804]	-1.227 [-1.670, -0.789]	0.922 [0.861, 0.963]	0.710 [0.644, 0.801]
yc70m	PCM/B3LYP/6-311+G(d,p)	1.878 [1.595, 2.153]	1.674 [1.369, 1.985]	0.688 [0.027, 1.300]	0.531 [0.332, 0.723]	0.793 [0.575, 1.077]
5byn6	Adiabatic scheme for type III submission	1.891 [1.489, 2.271]	1.553 [1.179, 1.945]	-1.273 [-1.770, -0.770]	0.912 [0.841, 0.957]	0.677 [0.613, 0.759]
y75vj	Direct scheme for type III submission	1.901 [1.504, 2.259]	1.584 [1.215, 1.966]	-1.039 [-1.611, -0.466]	0.891 [0.790, 0.952]	0.663 [0.597, 0.734]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.219, 2.705]	1.435 [1.037, 1.938]	0.467 [-0.224, 1.076]	0.709 [0.602, 0.869]	0.655 [0.474, 0.976]
w4iyd	Vertical scheme for type III submission	1.939 [1.531, 2.307]	1.578 [1.186, 1.995]	-1.211 [-1.753, -0.667]	0.849 [0.713, 0.928]	0.676 [0.600, 0.773]
pwn3m	Analog_search	1.970 [0.764, 2.846]	1.115 [0.562, 1.805]	-0.285 [-1.086, 0.373]	0.354 [0.015, 0.896]	0.607 [0.113, 0.870]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.376, 2.955]	1.578 [1.098, 2.153]	0.733 [-0.043, 1.417]	0.769 [0.668, 0.891]	0.596 [0.455, 0.815]
xikp8	Direct scheme with single point correction for...	2.340 [1.914, 2.734]	2.026 [1.610, 2.462]	-0.933 [-1.691, -0.135]	0.867 [0.768, 0.933]	0.569 [0.492, 0.650]
5nm4j	Substructure matches from experimental data	2.450 [1.416, 3.338]	1.583 [0.939, 2.336]	-0.046 [-1.024, 0.804]	0.192 [0.002, 0.695]	0.484 [-0.086, 0.967]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.508 [1.618, 3.294]	1.744 [1.146, 2.424]	0.526 [-0.373, 1.401]	0.726 [0.595, 0.849]	0.528 [0.402, 0.717]
0hxtm	COSMOtherm_FINE17	2.638 [0.868, 3.833]	1.423 [0.658, 2.389]	-0.736 [-1.822, 0.138]	0.127 [0.000, 0.832]	0.313 [-0.207, 0.778]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.987 [1.456, 4.611]	1.883 [1.241, 2.831]	0.230 [-0.705, 1.430]	0.540 [0.243, 0.881]	0.461 [0.229, 0.747]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	2.989 [1.284, 4.718]	1.695 [1.012, 2.707]	0.773 [-0.123, 1.961]	0.516 [0.219, 0.884]	0.450 [0.208, 0.771]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	3.007 [1.458, 4.639]	1.841 [1.174, 2.818]	0.491 [-0.410, 1.671]	0.547 [0.251, 0.874]	0.459 [0.234, 0.742]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	3.277 [1.488, 5.062]	1.985 [1.236, 3.070]	0.102 [-0.945, 1.389]	0.523 [0.229, 0.870]	0.404 [0.195, 0.703]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	3.288 [1.496, 5.070]	1.997 [1.251, 3.072]	0.138 [-0.918, 1.413]	0.526 [0.238, 0.874]	0.403 [0.198, 0.695]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	4.111 [1.887, 6.420]	2.443 [1.516, 3.832]	0.470 [-0.797, 2.082]	0.486 [0.196, 0.879]	0.339 [0.151, 0.626]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	4.558 [2.422, 6.850]	2.999 [1.990, 4.391]	0.370 [-1.118, 2.114]	0.517 [0.226, 0.879]	0.315 [0.150, 0.542]

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-sequential method (submission ID: nb007) were not blind. They were submitted after the submission deadline to be used as a reference method.