ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.544, 0.813]	0.579 [0.450, 0.712]	-0.235 [-0.459, 0.002]	0.937 [0.876, 0.973]	1.015 [0.913, 1.115]
gyuhx	S+pKa	0.732 [0.557, 0.912]	0.585 [0.438, 0.745]	-0.035 [-0.282, 0.226]	0.929 [0.879, 0.966]	0.948 [0.837, 1.047]
xmyhm	ACD/pKa Classic	0.787 [0.515, 1.033]	0.564 [0.382, 0.767]	-0.134 [-0.401, 0.142]	0.919 [0.848, 0.968]	0.956 [0.841, 1.068]
nb007	Epik-sequential	0.968 [0.767, 1.167]	0.810 [0.631, 0.997]	-0.025 [-0.354, 0.322]	0.871 [0.768, 0.934]	0.997 [0.857, 1.118]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.785, 1.353]	0.814 [0.584, 1.062]	0.475 [0.145, 0.814]	0.906 [0.839, 0.952]	0.840 [0.748, 0.956]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.087 [0.738, 1.447]	0.799 [0.561, 1.074]	0.166 [-0.227, 0.520]	0.846 [0.721, 0.942]	0.924 [0.799, 1.079]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.428, 1.720]	0.924 [0.128, 1.720]	0.910 [0.522, 1.000]	0.768 [0.558, 1.516]
37xm8	ACD/pKa GALAS	1.413 [0.928, 1.845]	1.008 [0.681, 1.382]	0.183 [-0.311, 0.692]	0.834 [0.701, 0.926]	0.721 [0.590, 0.868]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.141, 2.042]	1.239 [0.908, 1.613]	0.316 [-0.218, 0.886]	0.803 [0.665, 0.904]	0.705 [0.568, 0.836]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.196, 2.067]	1.296 [0.956, 1.669]	0.122 [-0.443, 0.700]	0.813 [0.686, 0.908]	0.678 [0.549, 0.802]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.060, 2.374]	1.213 [0.847, 1.671]	-0.442 [-1.053, 0.091]	0.797 [0.697, 0.899]	0.689 [0.537, 0.882]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.080, 2.363]	1.246 [0.888, 1.684]	-0.509 [-1.093, 0.037]	0.796 [0.697, 0.899]	0.690 [0.541, 0.887]
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 [0.434, 0.806]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.308, 2.248]	1.389 [1.015, 1.803]	0.744 [0.158, 1.315]	0.792 [0.656, 0.894]	0.689 [0.556, 0.848]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.390, 2.221]	1.482 [1.124, 1.863]	-0.103 [-0.734, 0.556]	0.820 [0.704, 0.907]	0.634 [0.517, 0.747]
ryzue	Adiabatic scheme with single point correction ...	1.824 [1.431, 2.190]	1.500 [1.147, 1.878]	-1.298 [-1.750, -0.845]	0.892 [0.825, 0.953]	0.733 [0.657, 0.851]
5byn6	Adiabatic scheme for type III submission	1.890 [1.498, 2.257]	1.588 [1.235, 1.958]	-1.317 [-1.794, -0.834]	0.905 [0.849, 0.948]	0.705 [0.627, 0.802]
y75vj	Direct scheme for type III submission	1.901 [1.493, 2.268]	1.584 [1.214, 1.974]	-1.039 [-1.608, -0.471]	0.891 [0.789, 0.950]	0.663 [0.598, 0.735]
w4iyd	Vertical scheme for type III submission	1.926 [1.523, 2.286]	1.584 [1.199, 1.987]	-1.257 [-1.774, -0.737]	0.853 [0.741, 0.921]	0.707 [0.622, 0.817]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.209, 2.697]	1.435 [1.035, 1.933]	0.467 [-0.232, 1.085]	0.709 [0.602, 0.870]	0.655 [0.476, 0.975]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.383, 2.646]	1.568 [1.171, 2.064]	-0.557 [-1.244, 0.112]	0.823 [0.722, 0.902]	0.610 [0.496, 0.735]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.380, 2.651]	1.577 [1.175, 2.071]	-0.524 [-1.250, 0.133]	0.825 [0.724, 0.905]	0.607 [0.499, 0.737]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.053 [1.706, 2.391]	1.805 [1.459, 2.144]	0.405 [-0.313, 1.076]	0.460 [0.267, 0.647]	0.831 [0.622, 1.129]
hytjn	OE Gaussian Process	2.161 [1.250, 3.090]	1.389 [0.855, 2.033]	-0.709 [-1.495, -0.017]	0.449 [0.123, 0.783]	0.723 [0.464, 0.899]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.364, 2.940]	1.578 [1.090, 2.152]	0.733 [-0.021, 1.424]	0.769 [0.669, 0.890]	0.596 [0.458, 0.813]
q3pfp	OE Gaussian Process Resampled	2.193 [1.323, 3.054]	1.505 [0.994, 2.114]	-0.589 [-1.404, 0.112]	0.443 [0.130, 0.766]	0.674 [0.442, 0.849]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.600, 2.807]	1.778 [1.328, 2.268]	-0.784 [-1.515, -0.066]	0.822 [0.696, 0.906]	0.584 [0.486, 0.692]
xikp8	Direct scheme with single point correction for...	2.348 [1.930, 2.731]	2.056 [1.653, 2.466]	-0.773 [-1.555, 0.032]	0.890 [0.797, 0.946]	0.560 [0.496, 0.625]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.795, 2.933]	1.915 [1.445, 2.425]	-0.313 [-1.134, 0.503]	0.842 [0.745, 0.913]	0.540 [0.452, 0.635]
5nm4j	Substructure matches from experimental data	2.450 [1.426, 3.341]	1.583 [0.941, 2.349]	-0.046 [-1.014, 0.804]	0.192 [0.002, 0.694]	0.484 [-0.087, 0.962]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.689, 3.301]	1.826 [1.256, 2.479]	0.651 [-0.246, 1.479]	0.761 [0.631, 0.877]	0.532 [0.418, 0.697]
pwn3m	Analog_search	2.604 [1.443, 3.514]	1.539 [0.831, 2.364]	-0.788 [-1.758, 0.061]	0.208 [0.003, 0.631]	0.563 [-0.005, 0.869]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.361, 3.564]	2.525 [1.964, 3.095]	-0.424 [-1.485, 0.575]	0.844 [0.739, 0.917]	0.473 [0.397, 0.547]
0hxtm	COSMOtherm_FINE17	3.371 [1.865, 4.556]	1.918 [0.980, 2.993]	-1.377 [-2.561, -0.328]	0.046 [0.000, 0.453]	0.211 [-0.254, 0.612]

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