ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.543, 0.809]	0.579 [0.449, 0.710]	-0.235 [-0.460, 0.008]	0.937 [0.877, 0.972]	1.015 [0.914, 1.114]
gyuhx	S+pKa	0.732 [0.555, 0.911]	0.585 [0.438, 0.744]	-0.035 [-0.284, 0.233]	0.929 [0.878, 0.965]	0.948 [0.833, 1.045]
xmyhm	ACD/pKa Classic	0.787 [0.521, 1.032]	0.564 [0.384, 0.771]	-0.134 [-0.400, 0.143]	0.919 [0.844, 0.968]	0.956 [0.839, 1.067]
nb007	Epik-sequential	0.968 [0.764, 1.172]	0.810 [0.626, 1.002]	-0.025 [-0.362, 0.313]	0.871 [0.761, 0.933]	0.997 [0.852, 1.118]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.782, 1.356]	0.814 [0.582, 1.072]	0.475 [0.143, 0.823]	0.906 [0.840, 0.952]	0.840 [0.747, 0.956]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.087 [0.730, 1.448]	0.799 [0.558, 1.071]	0.166 [-0.239, 0.517]	0.846 [0.721, 0.943]	0.924 [0.803, 1.088]
p0jba	macroscopic pKa prediction from microscopic pK...	1.315 [0.687, 1.728]	1.084 [0.428, 1.720]	0.924 [0.108, 1.720]	0.910 [0.509, 1.000]	0.768 [0.558, 1.516]
37xm8	ACD/pKa GALAS	1.413 [0.930, 1.844]	1.008 [0.681, 1.383]	0.183 [-0.319, 0.688]	0.834 [0.695, 0.927]	0.721 [0.588, 0.863]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.143, 2.035]	1.239 [0.912, 1.610]	0.316 [-0.229, 0.875]	0.803 [0.671, 0.903]	0.705 [0.568, 0.834]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.199, 2.074]	1.296 [0.960, 1.675]	0.122 [-0.447, 0.706]	0.813 [0.681, 0.909]	0.678 [0.549, 0.800]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.064, 2.376]	1.213 [0.855, 1.675]	-0.442 [-1.046, 0.113]	0.797 [0.702, 0.897]	0.689 [0.539, 0.884]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.074, 2.369]	1.246 [0.881, 1.692]	-0.509 [-1.124, 0.035]	0.796 [0.696, 0.896]	0.690 [0.542, 0.884]
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 [0.457, 1.000]	0.635 [0.394, 0.806]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.292, 2.254]	1.389 [1.002, 1.811]	0.744 [0.159, 1.307]	0.792 [0.653, 0.894]	0.689 [0.552, 0.852]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.386, 2.230]	1.482 [1.127, 1.871]	-0.103 [-0.721, 0.561]	0.820 [0.704, 0.906]	0.634 [0.519, 0.748]
ryzue	Adiabatic scheme with single point correction ...	1.824 [1.439, 2.180]	1.500 [1.147, 1.873]	-1.298 [-1.738, -0.840]	0.892 [0.826, 0.954]	0.733 [0.658, 0.847]
5byn6	Adiabatic scheme for type III submission	1.890 [1.500, 2.257]	1.588 [1.242, 1.953]	-1.317 [-1.786, -0.837]	0.905 [0.849, 0.948]	0.705 [0.629, 0.807]
y75vj	Direct scheme for type III submission	1.901 [1.498, 2.263]	1.584 [1.213, 1.960]	-1.039 [-1.596, -0.460]	0.891 [0.790, 0.951]	0.663 [0.598, 0.737]
w4iyd	Vertical scheme for type III submission	1.926 [1.531, 2.275]	1.584 [1.205, 1.969]	-1.257 [-1.764, -0.721]	0.853 [0.743, 0.922]	0.707 [0.622, 0.817]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.210, 2.726]	1.435 [1.033, 1.941]	0.467 [-0.241, 1.089]	0.709 [0.604, 0.867]	0.655 [0.475, 0.966]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.381, 2.656]	1.568 [1.169, 2.041]	-0.557 [-1.287, 0.094]	0.823 [0.720, 0.902]	0.610 [0.496, 0.737]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.392, 2.648]	1.577 [1.180, 2.051]	-0.524 [-1.228, 0.144]	0.825 [0.722, 0.904]	0.607 [0.497, 0.732]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.053 [1.710, 2.404]	1.805 [1.471, 2.156]	0.405 [-0.336, 1.072]	0.460 [0.272, 0.646]	0.831 [0.625, 1.121]
hytjn	OE Gaussian Process	2.161 [1.240, 3.071]	1.389 [0.846, 2.024]	-0.709 [-1.474, -0.006]	0.449 [0.129, 0.780]	0.723 [0.470, 0.901]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.386, 2.947]	1.578 [1.096, 2.157]	0.733 [-0.034, 1.419]	0.769 [0.672, 0.892]	0.596 [0.457, 0.811]
q3pfp	OE Gaussian Process Resampled	2.193 [1.337, 3.087]	1.505 [0.997, 2.138]	-0.589 [-1.404, 0.119]	0.443 [0.126, 0.771]	0.674 [0.440, 0.854]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.624, 2.809]	1.778 [1.344, 2.267]	-0.784 [-1.528, -0.078]	0.822 [0.695, 0.905]	0.584 [0.484, 0.688]
xikp8	Direct scheme with single point correction for...	2.348 [1.938, 2.720]	2.056 [1.661, 2.469]	-0.773 [-1.567, 0.020]	0.890 [0.795, 0.946]	0.560 [0.497, 0.624]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.792, 2.942]	1.915 [1.441, 2.438]	-0.313 [-1.142, 0.513]	0.842 [0.738, 0.912]	0.540 [0.452, 0.639]
5nm4j	Substructure matches from experimental data	2.450 [1.418, 3.338]	1.583 [0.931, 2.325]	-0.046 [-1.046, 0.800]	0.192 [0.002, 0.693]	0.484 [-0.065, 0.960]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.657, 3.304]	1.826 [1.241, 2.482]	0.651 [-0.247, 1.473]	0.761 [0.631, 0.877]	0.532 [0.420, 0.697]
pwn3m	Analog_search	2.604 [1.462, 3.522]	1.539 [0.830, 2.377]	-0.788 [-1.758, 0.056]	0.208 [0.003, 0.628]	0.563 [0.001, 0.875]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.357, 3.565]	2.525 [1.983, 3.099]	-0.424 [-1.470, 0.617]	0.844 [0.736, 0.917]	0.473 [0.396, 0.549]
0hxtm	COSMOtherm_FINE17	3.371 [1.865, 4.555]	1.918 [0.980, 3.024]	-1.377 [-2.579, -0.326]	0.046 [0.000, 0.453]	0.211 [-0.260, 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.