ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.548, 0.809]	0.579 [0.453, 0.709]	-0.235 [-0.459, 0.002]	0.937 [0.878, 0.972]	1.015 [0.911, 1.116]
gyuhx	S+pKa	0.732 [0.555, 0.908]	0.585 [0.435, 0.749]	-0.035 [-0.286, 0.234]	0.929 [0.879, 0.965]	0.948 [0.836, 1.045]
xmyhm	ACD/pKa Classic	0.787 [0.518, 1.032]	0.564 [0.383, 0.772]	-0.134 [-0.404, 0.141]	0.919 [0.846, 0.968]	0.956 [0.839, 1.068]
nb007	Epik-sequential	0.968 [0.762, 1.175]	0.810 [0.630, 1.008]	-0.025 [-0.356, 0.326]	0.871 [0.768, 0.935]	0.997 [0.858, 1.117]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.779, 1.356]	0.814 [0.579, 1.063]	0.475 [0.137, 0.815]	0.906 [0.842, 0.952]	0.840 [0.746, 0.956]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.087 [0.730, 1.460]	0.799 [0.558, 1.080]	0.166 [-0.232, 0.524]	0.846 [0.720, 0.944]	0.924 [0.796, 1.087]
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, 1.855]	1.008 [0.681, 1.389]	0.183 [-0.328, 0.679]	0.834 [0.694, 0.926]	0.721 [0.586, 0.867]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.140, 2.048]	1.239 [0.909, 1.623]	0.316 [-0.220, 0.883]	0.803 [0.672, 0.904]	0.705 [0.566, 0.835]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.200, 2.059]	1.296 [0.959, 1.662]	0.122 [-0.445, 0.719]	0.813 [0.686, 0.908]	0.678 [0.553, 0.803]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.055, 2.358]	1.213 [0.848, 1.668]	-0.442 [-1.044, 0.094]	0.797 [0.700, 0.899]	0.689 [0.540, 0.886]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.078, 2.383]	1.246 [0.887, 1.691]	-0.509 [-1.107, 0.034]	0.796 [0.697, 0.896]	0.690 [0.541, 0.883]
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]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.300, 2.246]	1.389 [1.009, 1.806]	0.744 [0.172, 1.300]	0.792 [0.660, 0.893]	0.689 [0.553, 0.852]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.384, 2.223]	1.482 [1.122, 1.871]	-0.103 [-0.738, 0.539]	0.820 [0.701, 0.906]	0.634 [0.519, 0.750]
ryzue	Adiabatic scheme with single point correction ...	1.824 [1.429, 2.177]	1.500 [1.148, 1.866]	-1.298 [-1.740, -0.847]	0.892 [0.824, 0.955]	0.733 [0.655, 0.849]
5byn6	Adiabatic scheme for type III submission	1.890 [1.497, 2.259]	1.588 [1.230, 1.958]	-1.317 [-1.789, -0.839]	0.905 [0.851, 0.948]	0.705 [0.630, 0.810]
y75vj	Direct scheme for type III submission	1.901 [1.502, 2.258]	1.584 [1.221, 1.966]	-1.039 [-1.611, -0.468]	0.891 [0.788, 0.950]	0.663 [0.597, 0.737]
w4iyd	Vertical scheme for type III submission	1.926 [1.529, 2.283]	1.584 [1.209, 1.977]	-1.257 [-1.775, -0.740]	0.853 [0.740, 0.923]	0.707 [0.622, 0.820]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.208, 2.719]	1.435 [1.026, 1.943]	0.467 [-0.236, 1.079]	0.709 [0.601, 0.869]	0.655 [0.474, 0.977]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.376, 2.630]	1.568 [1.163, 2.035]	-0.557 [-1.244, 0.098]	0.823 [0.724, 0.904]	0.610 [0.500, 0.738]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.385, 2.655]	1.577 [1.174, 2.053]	-0.524 [-1.231, 0.144]	0.825 [0.720, 0.904]	0.607 [0.497, 0.735]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.053 [1.709, 2.402]	1.805 [1.470, 2.161]	0.405 [-0.333, 1.091]	0.460 [0.268, 0.646]	0.831 [0.626, 1.126]
hytjn	OE Gaussian Process	2.161 [1.254, 3.070]	1.389 [0.870, 2.043]	-0.709 [-1.490, -0.023]	0.449 [0.128, 0.782]	0.723 [0.472, 0.898]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.364, 2.943]	1.578 [1.092, 2.152]	0.733 [-0.031, 1.427]	0.769 [0.667, 0.894]	0.596 [0.456, 0.816]
q3pfp	OE Gaussian Process Resampled	2.193 [1.330, 3.075]	1.505 [0.998, 2.131]	-0.589 [-1.376, 0.110]	0.443 [0.126, 0.767]	0.674 [0.441, 0.852]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.615, 2.811]	1.778 [1.335, 2.272]	-0.784 [-1.532, -0.073]	0.822 [0.697, 0.906]	0.584 [0.487, 0.689]
xikp8	Direct scheme with single point correction for...	2.348 [1.935, 2.734]	2.056 [1.657, 2.482]	-0.773 [-1.549, 0.029]	0.890 [0.798, 0.946]	0.560 [0.495, 0.623]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.801, 2.952]	1.915 [1.450, 2.434]	-0.313 [-1.168, 0.511]	0.842 [0.744, 0.914]	0.540 [0.451, 0.635]
5nm4j	Substructure matches from experimental data	2.450 [1.417, 3.341]	1.583 [0.937, 2.333]	-0.046 [-1.028, 0.810]	0.192 [0.002, 0.696]	0.484 [-0.078, 0.971]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.683, 3.303]	1.826 [1.249, 2.474]	0.651 [-0.264, 1.475]	0.761 [0.632, 0.875]	0.532 [0.417, 0.696]
pwn3m	Analog_search	2.604 [1.445, 3.524]	1.539 [0.829, 2.366]	-0.788 [-1.776, 0.056]	0.208 [0.004, 0.628]	0.563 [-0.001, 0.872]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.353, 3.576]	2.525 [1.974, 3.111]	-0.424 [-1.447, 0.625]	0.844 [0.739, 0.917]	0.473 [0.397, 0.550]
0hxtm	COSMOtherm_FINE17	3.371 [1.884, 4.563]	1.918 [0.977, 3.004]	-1.377 [-2.577, -0.316]	0.046 [0.000, 0.451]	0.211 [-0.245, 0.617]

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.