ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.548, 0.809]	0.579 [0.454, 0.710]	0.235 [-0.006, 0.457]	0.937 [0.879, 0.973]	0.923 [0.840, 1.016]
gyuhx	S+pKa	0.732 [0.555, 0.915]	0.585 [0.436, 0.748]	0.035 [-0.233, 0.289]	0.929 [0.878, 0.965]	0.979 [0.904, 1.085]
xmyhm	ACD/pKa Classic	0.787 [0.526, 1.032]	0.564 [0.385, 0.767]	0.134 [-0.142, 0.408]	0.919 [0.845, 0.967]	0.961 [0.858, 1.080]
nb007	Epik Scan	0.946 [0.730, 1.161]	0.776 [0.594, 0.975]	0.045 [-0.305, 0.373]	0.879 [0.762, 0.945]	0.840 [0.767, 0.923]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.777, 1.235]	0.799 [0.585, 1.025]	-0.166 [-0.505, 0.195]	0.867 [0.783, 0.934]	0.927 [0.764, 1.082]
nb010	Epik Microscopic	1.028 [0.775, 1.265]	0.814 [0.602, 1.040]	0.243 [-0.112, 0.594]	0.869 [0.771, 0.939]	0.946 [0.827, 1.077]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.788, 1.358]	0.814 [0.580, 1.075]	-0.475 [-0.819, -0.143]	0.906 [0.841, 0.952]	1.078 [0.939, 1.221]
nb013	Jaguar	1.103 [0.709, 1.463]	0.803 [0.557, 1.079]	-0.148 [-0.549, 0.214]	0.884 [0.781, 0.947]	1.092 [0.907, 1.255]
nb015	Chemicalize v18.23 (ChemAxon MarvinSketch v18.23)	1.272 [0.990, 1.571]	1.044 [0.803, 1.311]	0.129 [-0.322, 0.559]	0.874 [0.799, 0.932]	1.162 [0.942, 1.338]
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 [0.355, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.922, 1.843]	1.008 [0.676, 1.381]	-0.183 [-0.685, 0.315]	0.834 [0.694, 0.927]	1.155 [0.978, 1.333]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.143, 2.050]	1.239 [0.910, 1.614]	-0.316 [-0.888, 0.228]	0.803 [0.666, 0.903]	1.140 [0.977, 1.338]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.215, 2.059]	1.296 [0.965, 1.663]	-0.122 [-0.711, 0.446]	0.813 [0.687, 0.907]	1.198 [1.029, 1.405]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.057, 2.350]	1.213 [0.849, 1.653]	0.442 [-0.094, 1.031]	0.797 [0.697, 0.900]	1.156 [0.954, 1.421]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.077, 2.403]	1.246 [0.885, 1.707]	0.509 [-0.042, 1.107]	0.796 [0.701, 0.895]	1.153 [0.948, 1.426]
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 [0.720, 2.147]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.425, 2.112]	1.500 [1.181, 1.839]	1.298 [0.868, 1.715]	0.910 [0.862, 0.949]	1.229 [1.058, 1.402]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.305, 2.246]	1.389 [1.009, 1.815]	-0.744 [-1.310, -0.161]	0.792 [0.655, 0.891]	1.149 [0.966, 1.372]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.389, 2.220]	1.482 [1.129, 1.864]	0.103 [-0.549, 0.717]	0.820 [0.703, 0.906]	1.294 [1.119, 1.504]
5byn6	Adiabatic scheme for type III submission	1.890 [1.497, 2.257]	1.588 [1.237, 1.950]	1.317 [0.819, 1.782]	0.905 [0.850, 0.947]	1.284 [1.102, 1.470]
y75vj	Direct scheme for type III submission	1.901 [1.502, 2.265]	1.584 [1.215, 1.973]	1.039 [0.464, 1.612]	0.891 [0.789, 0.950]	1.345 [1.161, 1.528]
w4iyd	Vertical scheme for type III submission	1.926 [1.536, 2.282]	1.584 [1.209, 1.976]	1.257 [0.736, 1.774]	0.853 [0.737, 0.922]	1.206 [1.003, 1.397]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.214, 2.745]	1.435 [1.035, 1.967]	-0.467 [-1.068, 0.259]	0.709 [0.601, 0.869]	1.083 [0.804, 1.439]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.375, 2.651]	1.568 [1.161, 2.053]	0.557 [-0.092, 1.278]	0.823 [0.723, 0.901]	1.350 [1.146, 1.608]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.389, 2.645]	1.577 [1.174, 2.046]	0.524 [-0.138, 1.237]	0.825 [0.721, 0.903]	1.358 [1.156, 1.609]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.721, 2.315]	1.805 [1.475, 2.125]	-0.405 [-1.083, 0.315]	0.469 [0.289, 0.644]	0.559 [0.353, 0.839]
hytjn	OE Gaussian Process	2.161 [1.260, 3.070]	1.389 [0.875, 2.037]	0.709 [0.030, 1.490]	0.449 [0.135, 0.781]	0.621 [0.266, 0.995]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.376, 2.952]	1.578 [1.090, 2.161]	-0.733 [-1.417, 0.035]	0.769 [0.667, 0.893]	1.291 [1.016, 1.638]
q3pfp	OE Gaussian Process Resampled	2.193 [1.325, 3.082]	1.505 [0.992, 2.131]	0.589 [-0.122, 1.379]	0.443 [0.128, 0.771]	0.658 [0.277, 1.062]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.616, 2.814]	1.778 [1.342, 2.274]	0.784 [0.066, 1.532]	0.822 [0.695, 0.906]	1.406 [1.202, 1.637]
xikp8	Direct scheme with single point correction for...	2.348 [1.941, 2.730]	2.056 [1.658, 2.470]	0.773 [-0.034, 1.551]	0.890 [0.796, 0.946]	1.588 [1.392, 1.809]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.795, 2.949]	1.915 [1.445, 2.440]	0.313 [-0.522, 1.155]	0.842 [0.741, 0.914]	1.557 [1.350, 1.823]
5nm4j	Substructure matches from experimental data	2.450 [1.407, 3.344]	1.583 [0.923, 2.333]	0.046 [-0.803, 1.059]	0.192 [0.002, 0.692]	0.398 [-0.069, 0.824]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.688, 3.294]	1.826 [1.264, 2.482]	-0.651 [-1.494, 0.246]	0.761 [0.631, 0.876]	1.432 [1.128, 1.778]
pwn3m	Analog_search	2.604 [1.441, 3.535]	1.539 [0.827, 2.375]	0.788 [-0.074, 1.768]	0.208 [0.004, 0.638]	0.369 [-0.003, 0.772]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.372, 3.572]	2.525 [1.977, 3.101]	0.424 [-0.610, 1.463]	0.844 [0.742, 0.916]	1.784 [1.553, 2.058]
0hxtm	COSMOtherm_FINE17	3.263 [1.765, 4.354]	1.918 [1.003, 2.948]	1.377 [0.349, 2.518]	0.075 [0.000, 0.495]	0.281 [-0.167, 0.856]

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.