ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.550, 0.811]	0.579 [0.453, 0.713]	0.235 [-0.002, 0.461]	0.937 [0.879, 0.972]	0.923 [0.837, 1.016]
gyuhx	S+pKa	0.732 [0.555, 0.909]	0.585 [0.436, 0.747]	0.035 [-0.234, 0.287]	0.929 [0.877, 0.965]	0.979 [0.903, 1.085]
xmyhm	ACD/pKa Classic	0.787 [0.524, 1.036]	0.564 [0.385, 0.772]	0.134 [-0.138, 0.400]	0.919 [0.847, 0.967]	0.961 [0.858, 1.082]
nb007	Epik-sequential	0.968 [0.759, 1.172]	0.810 [0.627, 1.000]	0.025 [-0.325, 0.363]	0.871 [0.764, 0.936]	0.874 [0.787, 0.978]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.779, 1.226]	0.799 [0.589, 1.025]	-0.166 [-0.505, 0.185]	0.867 [0.784, 0.934]	0.927 [0.768, 1.079]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.778, 1.362]	0.814 [0.578, 1.070]	-0.475 [-0.818, -0.142]	0.906 [0.841, 0.952]	1.078 [0.935, 1.218]
nb015	Chemicalize v18.23	1.272 [0.988, 1.569]	1.044 [0.800, 1.307]	0.129 [-0.337, 0.564]	0.874 [0.796, 0.933]	1.162 [0.939, 1.344]
nb014	Chemicalize v18.12	1.300 [1.014, 1.587]	1.073 [0.820, 1.348]	0.256 [-0.216, 0.690]	0.859 [0.793, 0.918]	1.127 [0.906, 1.330]
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 [0.339, 1.724]
37xm8	ACD/pKa GALAS	1.413 [0.929, 1.847]	1.008 [0.684, 1.389]	-0.183 [-0.688, 0.324]	0.834 [0.697, 0.927]	1.155 [0.980, 1.333]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.147, 2.044]	1.239 [0.912, 1.613]	-0.316 [-0.880, 0.224]	0.803 [0.667, 0.902]	1.140 [0.981, 1.337]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.200, 2.061]	1.296 [0.954, 1.668]	-0.122 [-0.711, 0.447]	0.813 [0.683, 0.908]	1.198 [1.026, 1.406]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.068, 2.348]	1.213 [0.855, 1.655]	0.442 [-0.094, 1.024]	0.797 [0.699, 0.897]	1.156 [0.954, 1.428]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.078, 2.374]	1.246 [0.880, 1.693]	0.509 [-0.027, 1.115]	0.796 [0.699, 0.895]	1.153 [0.949, 1.423]
35bdm	macroscopic pKa prediction from microscopic pK...	1.719 [0.665, 2.338]	1.442 [0.622, 2.262]	-1.006 [-2.178, 0.136]	0.919 [0.457, 1.000]	1.446 [0.720, 2.147]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.418, 2.112]	1.500 [1.173, 1.836]	1.298 [0.868, 1.716]	0.910 [0.861, 0.948]	1.229 [1.060, 1.402]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.298, 2.252]	1.389 [1.009, 1.808]	-0.744 [-1.303, -0.178]	0.792 [0.660, 0.892]	1.149 [0.961, 1.378]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.392, 2.229]	1.482 [1.130, 1.870]	0.103 [-0.546, 0.736]	0.820 [0.704, 0.906]	1.294 [1.116, 1.509]
5byn6	Adiabatic scheme for type III submission	1.890 [1.496, 2.271]	1.588 [1.231, 1.969]	1.317 [0.829, 1.796]	0.905 [0.847, 0.948]	1.284 [1.103, 1.461]
y75vj	Direct scheme for type III submission	1.901 [1.494, 2.264]	1.584 [1.217, 1.974]	1.039 [0.461, 1.603]	0.891 [0.792, 0.951]	1.345 [1.157, 1.531]
w4iyd	Vertical scheme for type III submission	1.926 [1.541, 2.275]	1.584 [1.207, 1.981]	1.257 [0.738, 1.761]	0.853 [0.738, 0.922]	1.206 [0.999, 1.404]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.219, 2.730]	1.435 [1.041, 1.951]	-0.467 [-1.072, 0.253]	0.709 [0.600, 0.870]	1.083 [0.810, 1.443]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.372, 2.639]	1.568 [1.163, 2.032]	0.557 [-0.094, 1.265]	0.823 [0.720, 0.904]	1.350 [1.146, 1.604]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.386, 2.640]	1.577 [1.177, 2.056]	0.524 [-0.141, 1.228]	0.825 [0.727, 0.904]	1.358 [1.160, 1.610]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.716, 2.322]	1.805 [1.463, 2.134]	-0.405 [-1.070, 0.319]	0.469 [0.291, 0.642]	0.559 [0.348, 0.834]
hytjn	OE Gaussian Process	2.161 [1.236, 3.096]	1.389 [0.851, 2.057]	0.709 [0.020, 1.493]	0.449 [0.130, 0.785]	0.621 [0.254, 1.000]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.383, 2.941]	1.578 [1.101, 2.150]	-0.733 [-1.415, 0.053]	0.769 [0.667, 0.892]	1.291 [1.020, 1.633]
q3pfp	OE Gaussian Process Resampled	2.193 [1.324, 3.076]	1.505 [0.987, 2.127]	0.589 [-0.130, 1.379]	0.443 [0.124, 0.774]	0.658 [0.273, 1.074]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.612, 2.816]	1.778 [1.339, 2.279]	0.784 [0.065, 1.519]	0.822 [0.693, 0.906]	1.406 [1.201, 1.628]
xikp8	Direct scheme with single point correction for...	2.348 [1.933, 2.721]	2.056 [1.657, 2.464]	0.773 [-0.031, 1.556]	0.890 [0.799, 0.947]	1.588 [1.394, 1.810]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.790, 2.942]	1.915 [1.437, 2.418]	0.313 [-0.513, 1.139]	0.842 [0.739, 0.914]	1.557 [1.349, 1.826]
5nm4j	Substructure matches from experimental data	2.450 [1.416, 3.361]	1.583 [0.932, 2.352]	0.046 [-0.804, 1.049]	0.192 [0.002, 0.692]	0.398 [-0.064, 0.816]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.653, 3.299]	1.826 [1.235, 2.488]	-0.651 [-1.495, 0.244]	0.761 [0.630, 0.875]	1.432 [1.121, 1.774]
pwn3m	Analog_search	2.604 [1.450, 3.520]	1.539 [0.829, 2.379]	0.788 [-0.057, 1.768]	0.208 [0.004, 0.626]	0.369 [0.004, 0.781]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.378, 3.578]	2.525 [1.983, 3.110]	0.424 [-0.607, 1.488]	0.844 [0.740, 0.917]	1.784 [1.556, 2.058]
0hxtm	COSMOtherm_FINE17	3.263 [1.785, 4.365]	1.918 [1.008, 2.948]	1.377 [0.362, 2.514]	0.075 [0.000, 0.477]	0.281 [-0.173, 0.840]

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.