ID	name	RMSE	MAE	ME	R^2	m
xvxzd	Full quantum chemical calculation of free ener...	0.680 [0.547, 0.811]	0.579 [0.453, 0.710]	0.235 [-0.004, 0.460]	0.937 [0.876, 0.973]	0.923 [0.836, 1.015]
gyuhx	S+pKa	0.732 [0.555, 0.908]	0.585 [0.436, 0.745]	0.035 [-0.235, 0.289]	0.929 [0.877, 0.965]	0.979 [0.903, 1.085]
xmyhm	ACD/pKa Classic	0.787 [0.528, 1.028]	0.564 [0.388, 0.766]	0.134 [-0.143, 0.409]	0.919 [0.845, 0.968]	0.961 [0.858, 1.083]
nb007	nb007-976-typeIII-epik_scan-1	0.946 [0.729, 1.151]	0.776 [0.593, 0.971]	0.045 [-0.302, 0.370]	0.879 [0.763, 0.945]	0.840 [0.768, 0.921]
yqkga	ReSCoSS conformations // COSMOtherm pKa	1.010 [0.777, 1.225]	0.799 [0.589, 1.019]	-0.166 [-0.505, 0.190]	0.867 [0.783, 0.935]	0.927 [0.762, 1.078]
nb010	nb010-976-typeIII-epik_microscopic-1	1.028 [0.766, 1.274]	0.814 [0.598, 1.049]	0.243 [-0.118, 0.587]	0.869 [0.770, 0.939]	0.946 [0.826, 1.079]
8xt50	ReSCoSS conformations // DSD-BLYP-D3 reranking...	1.071 [0.780, 1.371]	0.814 [0.582, 1.074]	-0.475 [-0.833, -0.145]	0.906 [0.840, 0.952]	1.078 [0.937, 1.217]
nb013	nb013-976-typeIII-jaguar-1	1.103 [0.703, 1.475]	0.803 [0.552, 1.093]	-0.148 [-0.555, 0.226]	0.884 [0.784, 0.947]	1.092 [0.904, 1.251]
nb015	Chemicalize v18.23	1.272 [0.988, 1.568]	1.044 [0.802, 1.310]	0.129 [-0.342, 0.559]	0.874 [0.799, 0.932]	1.162 [0.937, 1.340]
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 [0.933, 1.854]	1.008 [0.680, 1.395]	-0.183 [-0.689, 0.341]	0.834 [0.703, 0.927]	1.155 [0.979, 1.334]
mkhqa	EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par	1.596 [1.140, 2.045]	1.239 [0.907, 1.612]	-0.316 [-0.883, 0.218]	0.803 [0.669, 0.903]	1.140 [0.978, 1.344]
ttjd0	EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par	1.642 [1.195, 2.081]	1.296 [0.954, 1.677]	-0.122 [-0.718, 0.452]	0.813 [0.686, 0.909]	1.198 [1.029, 1.403]
nb001	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par	1.685 [1.059, 2.371]	1.213 [0.853, 1.674]	0.442 [-0.108, 1.052]	0.797 [0.701, 0.897]	1.156 [0.953, 1.430]
nb002	EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par	1.703 [1.087, 2.390]	1.246 [0.889, 1.711]	0.509 [-0.036, 1.106]	0.796 [0.698, 0.895]	1.153 [0.949, 1.425]
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 [0.457, 1.000]	1.446 [0.720, 2.147]
ryzue	Adiabatic scheme with single point correction ...	1.774 [1.410, 2.117]	1.500 [1.170, 1.844]	1.298 [0.865, 1.724]	0.910 [0.861, 0.948]	1.229 [1.055, 1.402]
2ii2g	EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par	1.795 [1.298, 2.250]	1.389 [1.005, 1.811]	-0.744 [-1.308, -0.165]	0.792 [0.662, 0.892]	1.149 [0.962, 1.367]
mpwiy	EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par	1.816 [1.395, 2.225]	1.482 [1.130, 1.869]	0.103 [-0.560, 0.727]	0.820 [0.701, 0.907]	1.294 [1.118, 1.506]
5byn6	Adiabatic scheme for type III submission	1.890 [1.508, 2.257]	1.588 [1.235, 1.954]	1.317 [0.839, 1.791]	0.905 [0.849, 0.948]	1.284 [1.105, 1.474]
y75vj	Direct scheme for type III submission	1.901 [1.493, 2.265]	1.584 [1.218, 1.970]	1.039 [0.445, 1.610]	0.891 [0.793, 0.952]	1.345 [1.162, 1.532]
w4iyd	Vertical scheme for type III submission	1.926 [1.528, 2.281]	1.584 [1.208, 1.970]	1.257 [0.733, 1.765]	0.853 [0.736, 0.922]	1.206 [1.002, 1.395]
np6b4	EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par	1.938 [1.217, 2.737]	1.435 [1.043, 1.958]	-0.467 [-1.075, 0.255]	0.709 [0.605, 0.866]	1.083 [0.807, 1.451]
nb004	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.009 [1.379, 2.644]	1.568 [1.170, 2.043]	0.557 [-0.108, 1.261]	0.823 [0.723, 0.903]	1.350 [1.147, 1.607]
nb003	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par	2.010 [1.384, 2.648]	1.577 [1.170, 2.062]	0.524 [-0.149, 1.245]	0.825 [0.724, 0.903]	1.358 [1.153, 1.613]
yc70m	PCM/B3LYP/6-311+G(d,p)	2.034 [1.725, 2.325]	1.805 [1.473, 2.136]	-0.405 [-1.089, 0.313]	0.469 [0.285, 0.647]	0.559 [0.350, 0.829]
hytjn	OE Gaussian Process	2.161 [1.249, 3.071]	1.389 [0.858, 2.027]	0.709 [0.021, 1.494]	0.449 [0.134, 0.780]	0.621 [0.269, 1.001]
f0gew	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par	2.184 [1.371, 2.959]	1.578 [1.093, 2.166]	-0.733 [-1.417, 0.051]	0.769 [0.666, 0.892]	1.291 [1.014, 1.638]
q3pfp	OE Gaussian Process Resampled	2.193 [1.334, 3.087]	1.505 [0.992, 2.134]	0.589 [-0.121, 1.396]	0.443 [0.125, 0.774]	0.658 [0.267, 1.072]
ds62k	EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par	2.218 [1.622, 2.826]	1.778 [1.339, 2.284]	0.784 [0.065, 1.546]	0.822 [0.698, 0.905]	1.406 [1.200, 1.632]
xikp8	Direct scheme with single point correction for...	2.348 [1.946, 2.719]	2.056 [1.662, 2.465]	0.773 [-0.047, 1.549]	0.890 [0.796, 0.946]	1.588 [1.396, 1.803]
nb005	EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par	2.378 [1.793, 2.956]	1.915 [1.438, 2.437]	0.313 [-0.502, 1.174]	0.842 [0.741, 0.913]	1.557 [1.344, 1.820]
5nm4j	Substructure matches from experimental data	2.450 [1.408, 3.328]	1.583 [0.938, 2.322]	0.046 [-0.801, 1.016]	0.192 [0.002, 0.699]	0.398 [-0.072, 0.825]
ad5pu	EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par	2.536 [1.657, 3.291]	1.826 [1.236, 2.469]	-0.651 [-1.497, 0.243]	0.761 [0.634, 0.876]	1.432 [1.129, 1.774]
pwn3m	Analog_search	2.604 [1.446, 3.530]	1.539 [0.823, 2.369]	0.788 [-0.064, 1.800]	0.208 [0.004, 0.624]	0.369 [0.008, 0.773]
nb006	EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par	2.982 [2.366, 3.571]	2.525 [1.991, 3.098]	0.424 [-0.608, 1.447]	0.844 [0.738, 0.916]	1.784 [1.557, 2.061]
0hxtm	COSMOtherm_FINE17	3.263 [1.794, 4.379]	1.918 [1.007, 2.976]	1.377 [0.345, 2.546]	0.075 [0.000, 0.487]	0.281 [-0.172, 0.845]

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.