| ID | name | RMSE | MAE | ME | $R^2$ | m |
|---|---|---|---|---|---|---|
| xvxzd | Full quantum chemical calculation of free ener... | 0.680 [0.546, 0.811] | 0.579 [0.450, 0.710] | -0.235 [-0.461, 0.001] | 0.937 [0.878, 0.972] | 1.015 [0.913, 1.115] |
| gyuhx | S+pKa | 0.730 [0.552, 0.916] | 0.579 [0.429, 0.749] | -0.009 [-0.265, 0.260] | 0.925 [0.868, 0.963] | 0.929 [0.814, 1.031] |
| xmyhm | ACD/pKa Classic | 0.774 [0.492, 1.034] | 0.546 [0.363, 0.761] | -0.102 [-0.370, 0.181] | 0.916 [0.829, 0.969] | 0.934 [0.818, 1.043] |
| yqkga | ReSCoSS conformations // COSMOtherm pKa | 0.903 [0.685, 1.117] | 0.710 [0.518, 0.919] | 0.288 [-0.026, 0.579] | 0.901 [0.821, 0.953] | 0.901 [0.776, 1.041] |
| nb007 | Epik-sequential | 0.968 [0.764, 1.175] | 0.810 [0.628, 1.005] | -0.025 [-0.357, 0.325] | 0.871 [0.762, 0.936] | 0.997 [0.858, 1.119] |
| 8xt50 | ReSCoSS conformations // DSD-BLYP-D3 reranking... | 1.071 [0.780, 1.356] | 0.814 [0.579, 1.070] | 0.475 [0.139, 0.822] | 0.906 [0.840, 0.951] | 0.840 [0.747, 0.957] |
| p0jba | macroscopic pKa prediction from microscopic pK... | 1.315 [0.687, 1.718] | 1.084 [0.428, 1.704] | 0.924 [0.108, 1.704] | 0.910 [0.509, 1.000] | 0.768 [0.558, 1.516] |
| 37xm8 | ACD/pKa GALAS | 1.358 [0.844, 1.811] | 0.955 [0.632, 1.331] | 0.101 [-0.400, 0.601] | 0.854 [0.730, 0.939] | 0.729 [0.599, 0.877] |
| hytjn | OE Gaussian Process | 1.434 [0.976, 1.832] | 1.034 [0.676, 1.422] | -0.240 [-0.778, 0.276] | 0.675 [0.420, 0.853] | 0.795 [0.601, 1.003] |
| q3pfp | OE Gaussian Process Resampled | 1.484 [1.049, 1.865] | 1.140 [0.808, 1.497] | -0.090 [-0.667, 0.445] | 0.667 [0.430, 0.837] | 0.752 [0.570, 0.968] |
| mkhqa | EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par | 1.596 [1.150, 2.037] | 1.239 [0.915, 1.612] | 0.316 [-0.222, 0.883] | 0.803 [0.670, 0.904] | 0.705 [0.569, 0.835] |
| 2ii2g | EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par | 1.683 [1.205, 2.131] | 1.304 [0.948, 1.695] | 1.061 [0.616, 1.535] | 0.837 [0.729, 0.916] | 0.780 [0.637, 0.925] |
| nb001 | EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par | 1.702 [1.063, 2.391] | 1.219 [0.842, 1.682] | -0.422 [-1.025, 0.144] | 0.792 [0.686, 0.898] | 0.664 [0.519, 0.856] |
| 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] |
| nb002 | EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par | 1.720 [1.080, 2.405] | 1.250 [0.875, 1.709] | -0.467 [-1.087, 0.104] | 0.794 [0.685, 0.900] | 0.662 [0.514, 0.850] |
| ryzue | Adiabatic scheme with single point correction ... | 1.745 [1.370, 2.101] | 1.436 [1.094, 1.804] | -1.227 [-1.670, -0.789] | 0.922 [0.861, 0.963] | 0.710 [0.644, 0.801] |
| yc70m | PCM/B3LYP/6-311+G(d,p) | 1.878 [1.595, 2.153] | 1.674 [1.369, 1.985] | 0.688 [0.027, 1.300] | 0.531 [0.332, 0.723] | 0.793 [0.575, 1.077] |
| 5byn6 | Adiabatic scheme for type III submission | 1.891 [1.489, 2.271] | 1.553 [1.179, 1.945] | -1.273 [-1.770, -0.770] | 0.912 [0.841, 0.957] | 0.677 [0.613, 0.759] |
| y75vj | Direct scheme for type III submission | 1.901 [1.504, 2.259] | 1.584 [1.215, 1.966] | -1.039 [-1.611, -0.466] | 0.891 [0.790, 0.952] | 0.663 [0.597, 0.734] |
| np6b4 | EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par | 1.938 [1.219, 2.705] | 1.435 [1.037, 1.938] | 0.467 [-0.224, 1.076] | 0.709 [0.602, 0.869] | 0.655 [0.474, 0.976] |
| w4iyd | Vertical scheme for type III submission | 1.939 [1.531, 2.307] | 1.578 [1.186, 1.995] | -1.211 [-1.753, -0.667] | 0.849 [0.713, 0.928] | 0.676 [0.600, 0.773] |
| pwn3m | Analog_search | 1.970 [0.764, 2.846] | 1.115 [0.562, 1.805] | -0.285 [-1.086, 0.373] | 0.354 [0.015, 0.896] | 0.607 [0.113, 0.870] |
| f0gew | EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par | 2.184 [1.376, 2.955] | 1.578 [1.098, 2.153] | 0.733 [-0.043, 1.417] | 0.769 [0.668, 0.891] | 0.596 [0.455, 0.815] |
| xikp8 | Direct scheme with single point correction for... | 2.340 [1.914, 2.734] | 2.026 [1.610, 2.462] | -0.933 [-1.691, -0.135] | 0.867 [0.768, 0.933] | 0.569 [0.492, 0.650] |
| 5nm4j | Substructure matches from experimental data | 2.450 [1.416, 3.338] | 1.583 [0.939, 2.336] | -0.046 [-1.024, 0.804] | 0.192 [0.002, 0.695] | 0.484 [-0.086, 0.967] |
| ad5pu | EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par | 2.508 [1.618, 3.294] | 1.744 [1.146, 2.424] | 0.526 [-0.373, 1.401] | 0.726 [0.595, 0.849] | 0.528 [0.402, 0.717] |
| 0hxtm | COSMOtherm_FINE17 | 2.638 [0.868, 3.833] | 1.423 [0.658, 2.389] | -0.736 [-1.822, 0.138] | 0.127 [0.000, 0.832] | 0.313 [-0.207, 0.778] |
| ds62k | EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par | 2.987 [1.456, 4.611] | 1.883 [1.241, 2.831] | 0.230 [-0.705, 1.430] | 0.540 [0.243, 0.881] | 0.461 [0.229, 0.747] |
| ttjd0 | EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par | 2.989 [1.284, 4.718] | 1.695 [1.012, 2.707] | 0.773 [-0.123, 1.961] | 0.516 [0.219, 0.884] | 0.450 [0.208, 0.771] |
| mpwiy | EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par | 3.007 [1.458, 4.639] | 1.841 [1.174, 2.818] | 0.491 [-0.410, 1.671] | 0.547 [0.251, 0.874] | 0.459 [0.234, 0.742] |
| nb004 | EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par | 3.277 [1.488, 5.062] | 1.985 [1.236, 3.070] | 0.102 [-0.945, 1.389] | 0.523 [0.229, 0.870] | 0.404 [0.195, 0.703] |
| nb003 | EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par | 3.288 [1.496, 5.070] | 1.997 [1.251, 3.072] | 0.138 [-0.918, 1.413] | 0.526 [0.238, 0.874] | 0.403 [0.198, 0.695] |
| nb005 | EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par | 4.111 [1.887, 6.420] | 2.443 [1.516, 3.832] | 0.470 [-0.797, 2.082] | 0.486 [0.196, 0.879] | 0.339 [0.151, 0.626] |
| nb006 | EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par | 4.558 [2.422, 6.850] | 2.999 [1.990, 4.391] | 0.370 [-1.118, 2.114] | 0.517 [0.226, 0.879] | 0.315 [0.150, 0.542] |

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.