| ID | name | RMSE | MAE | ME | $R^2$ | m |
|---|---|---|---|---|---|---|
| xvxzd | Full quantum chemical calculation of free ener... | 0.680 [0.547, 0.810] | 0.579 [0.451, 0.711] | -0.235 [-0.463, 0.004] | 0.937 [0.878, 0.973] | 1.015 [0.915, 1.113] |
| gyuhx | S+pKa | 0.730 [0.549, 0.912] | 0.579 [0.428, 0.740] | -0.009 [-0.264, 0.251] | 0.925 [0.868, 0.964] | 0.929 [0.812, 1.028] |
| xmyhm | ACD/pKa Classic | 0.774 [0.495, 1.032] | 0.546 [0.367, 0.757] | -0.102 [-0.372, 0.184] | 0.916 [0.829, 0.968] | 0.934 [0.815, 1.046] |
| yqkga | ReSCoSS conformations // COSMOtherm pKa | 0.903 [0.682, 1.121] | 0.710 [0.515, 0.917] | 0.288 [-0.030, 0.580] | 0.901 [0.826, 0.953] | 0.901 [0.773, 1.036] |
| nb007 | Epik-sequential | 0.968 [0.759, 1.171] | 0.810 [0.626, 1.001] | -0.025 [-0.358, 0.321] | 0.871 [0.762, 0.936] | 0.997 [0.853, 1.117] |
| 8xt50 | ReSCoSS conformations // DSD-BLYP-D3 reranking... | 1.071 [0.786, 1.362] | 0.814 [0.584, 1.073] | 0.475 [0.143, 0.823] | 0.906 [0.841, 0.951] | 0.840 [0.744, 0.954] |
| 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 | 1.358 [0.856, 1.806] | 0.955 [0.633, 1.330] | 0.101 [-0.388, 0.597] | 0.854 [0.729, 0.938] | 0.729 [0.600, 0.880] |
| hytjn | OE Gaussian Process | 1.434 [0.983, 1.829] | 1.034 [0.683, 1.418] | -0.240 [-0.755, 0.274] | 0.675 [0.413, 0.852] | 0.795 [0.601, 1.008] |
| q3pfp | OE Gaussian Process Resampled | 1.484 [1.056, 1.868] | 1.140 [0.808, 1.508] | -0.090 [-0.656, 0.427] | 0.667 [0.436, 0.837] | 0.752 [0.567, 0.963] |
| mkhqa | EC-RISM/MP2/cc-pVTZ-P2-phi-all-2par | 1.596 [1.134, 2.041] | 1.239 [0.906, 1.619] | 0.316 [-0.222, 0.890] | 0.803 [0.671, 0.903] | 0.705 [0.567, 0.837] |
| 2ii2g | EC-RISM/MP2/cc-pVTZ-P2-q-noThiols-2par | 1.683 [1.202, 2.158] | 1.304 [0.956, 1.725] | 1.061 [0.615, 1.553] | 0.837 [0.733, 0.915] | 0.780 [0.637, 0.927] |
| nb001 | EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par | 1.702 [1.055, 2.389] | 1.219 [0.837, 1.672] | -0.422 [-1.033, 0.134] | 0.792 [0.685, 0.899] | 0.664 [0.517, 0.858] |
| 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 [1.077, 2.399] | 1.250 [0.878, 1.719] | -0.467 [-1.087, 0.092] | 0.794 [0.687, 0.902] | 0.662 [0.516, 0.850] |
| ryzue | Adiabatic scheme with single point correction ... | 1.745 [1.358, 2.091] | 1.436 [1.087, 1.790] | -1.227 [-1.659, -0.773] | 0.922 [0.861, 0.962] | 0.710 [0.642, 0.795] |
| yc70m | PCM/B3LYP/6-311+G(d,p) | 1.878 [1.587, 2.148] | 1.674 [1.359, 1.982] | 0.688 [0.028, 1.304] | 0.531 [0.333, 0.721] | 0.793 [0.581, 1.065] |
| 5byn6 | Adiabatic scheme for type III submission | 1.891 [1.491, 2.271] | 1.553 [1.183, 1.940] | -1.273 [-1.763, -0.785] | 0.912 [0.841, 0.959] | 0.677 [0.613, 0.760] |
| y75vj | Direct scheme for type III submission | 1.901 [1.504, 2.254] | 1.584 [1.216, 1.962] | -1.039 [-1.596, -0.473] | 0.891 [0.790, 0.950] | 0.663 [0.596, 0.736] |
| np6b4 | EC-RISM/B3LYP/6-311+G(d,p)-P2-phi-noThiols-2par | 1.938 [1.212, 2.726] | 1.435 [1.038, 1.945] | 0.467 [-0.235, 1.072] | 0.709 [0.600, 0.868] | 0.655 [0.475, 0.975] |
| w4iyd | Vertical scheme for type III submission | 1.939 [1.531, 2.316] | 1.578 [1.174, 2.004] | -1.211 [-1.756, -0.666] | 0.849 [0.715, 0.930] | 0.676 [0.602, 0.773] |
| pwn3m | Analog_search | 1.970 [0.773, 2.860] | 1.115 [0.566, 1.816] | -0.285 [-1.112, 0.376] | 0.354 [0.018, 0.901] | 0.607 [0.133, 0.869] |
| f0gew | EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par | 2.184 [1.394, 2.937] | 1.578 [1.103, 2.148] | 0.733 [-0.029, 1.416] | 0.769 [0.665, 0.892] | 0.596 [0.454, 0.811] |
| xikp8 | Direct scheme with single point correction for... | 2.340 [1.912, 2.731] | 2.026 [1.610, 2.458] | -0.933 [-1.703, -0.144] | 0.867 [0.768, 0.933] | 0.569 [0.492, 0.649] |
| 5nm4j | Substructure matches from experimental data | 2.450 [1.417, 3.336] | 1.583 [0.938, 2.333] | -0.046 [-1.053, 0.810] | 0.192 [0.001, 0.697] | 0.484 [-0.099, 0.961] |
| ad5pu | EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par | 2.508 [1.602, 3.287] | 1.744 [1.143, 2.420] | 0.526 [-0.373, 1.379] | 0.726 [0.591, 0.850] | 0.528 [0.403, 0.724] |
| 0hxtm | COSMOtherm_FINE17 | 2.638 [0.881, 3.820] | 1.423 [0.666, 2.372] | -0.736 [-1.794, 0.136] | 0.127 [0.001, 0.835] | 0.313 [-0.199, 0.777] |
| ds62k | EC-RISM/MP2/6-311+G(d,p)-P3NI-q-noThiols-2par | 2.987 [1.454, 4.609] | 1.883 [1.243, 2.835] | 0.230 [-0.715, 1.408] | 0.540 [0.241, 0.882] | 0.461 [0.226, 0.747] |
| ttjd0 | EC-RISM/MP2/cc-pVTZ-P2-phi-noThiols-2par | 2.989 [1.293, 4.723] | 1.695 [1.015, 2.737] | 0.773 [-0.094, 1.936] | 0.516 [0.222, 0.882] | 0.450 [0.210, 0.776] |
| mpwiy | EC-RISM/MP2/cc-pVTZ-P3NI-phi-noThiols-2par | 3.007 [1.451, 4.626] | 1.841 [1.164, 2.795] | 0.491 [-0.420, 1.644] | 0.547 [0.247, 0.876] | 0.459 [0.230, 0.740] |
| nb004 | EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-noThiols-2par | 3.277 [1.483, 5.066] | 1.985 [1.229, 3.075] | 0.102 [-0.932, 1.400] | 0.523 [0.227, 0.870] | 0.404 [0.190, 0.705] |
| nb003 | EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-2par | 3.288 [1.474, 5.085] | 1.997 [1.232, 3.078] | 0.138 [-0.904, 1.445] | 0.526 [0.233, 0.875] | 0.403 [0.195, 0.703] |
| nb005 | EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par | 4.111 [1.875, 6.415] | 2.443 [1.511, 3.806] | 0.470 [-0.829, 2.053] | 0.486 [0.194, 0.879] | 0.339 [0.152, 0.631] |
| nb006 | EC-RISM/MP2/6-311+G(d,p)-P3NI-phi-all-1par | 4.558 [2.439, 6.850] | 2.999 [2.017, 4.388] | 0.370 [-1.099, 2.135] | 0.517 [0.226, 0.881] | 0.315 [0.151, 0.543] |

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.