| ID | name | RMSE | MAE | ME | $R^2$ | m | |
|---|---|---|---|---|---|---|---|
| hmz0n | cosmotherm_FINE19 | 0.38 [0.23, 0.55] | 0.31 [0.19, 0.47] | -0.17 [-0.39, 0.03] | 0.77 [0.33, 0.94] | 0.94 [0.59, 1.16] | 0.64 [ |
| 1.15 [0.91, 1.34] | | | | | | | |
| gmoq5 | Global XGBoost-Based QSPR LogP Predictor | 0.39 [0.27, 0.48] | 0.34 [0.23, 0.46] | 0.01 [-0.22, 0.25] | 0.74 [0.38, 0.93] | 0.99 [0.65, 1.34] | 0.59 [ |
| 0.69 [0.39, 1.02] | | | | | | | |
| 3vqbi | cosmoquick_TZVP18+ML | 0.41 [0.29, 0.52] | 0.36 [0.25, 0.48] | -0.08 [-0.28, 0.17] | 0.66 [0.25, 0.93] | 0.78 [0.48, 1.04] | 0.56 [ |
| 1.06 [0.84, 1.24] | | | | | | | |
| j8nwc | EC_RISM_wet_P1w+2o | 0.47 [0.16, 0.75] | 0.31 [0.15, 0.55] | 0.07 [-0.16, 0.38] | 0.74 [0.28, 0.97] | 1.14 [0.82, 1.38] | 0.81 [ |
| 1.31 [1.06, 1.47] | | | | | | | |
| sq07q | Local XGBoost-Based QSPR LogP Predictor | 0.47 [0.34, 0.58] | 0.41 [0.28, 0.54] | 0.03 [-0.25, 0.31] | 0.64 [0.24, 0.88] | 0.92 [0.52, 1.33] | 0.56 [ |
| 0.60 [0.29, 0.93] | | | | | | | |
| dqxk4 | LogP_SMD_Solvation_DFT | 0.49 [0.33, 0.64] | 0.42 [0.26, 0.59] | 0.30 [0.07, 0.55] | 0.69 [0.34, 0.92] | 0.83 [0.49, 1.26] | 0.67 [ |
| 1.13 [0.94, 1.31] | | | | | | | |
| xxh4i | SM12-Solvation-Trained | 0.49 [0.34, 0.62] | 0.43 [0.29, 0.58] | 0.18 [-0.11, 0.44] | 0.54 [0.13, 0.86] | 0.60 [0.31, 1.04] | 0.51 [ |
| 1.41 [1.35, 1.46] | | | | | | | |
| hdpuj | RayLogP-II, a cheminformatic QSPR model predic... | 0.49 [0.36, 0.61] | 0.44 [0.32, 0.58] | -0.29 [-0.51, -0.05] | 0.74 [0.38, 0.95] | 1.02 [0.68, 1.37] | 0.67 [ |
| 0.91 [0.70, 1.14] | | | | | | | |
| vzgyt | rfs-logp | 0.50 [0.27, 0.68] | 0.38 [0.21, 0.59] | -0.35 [-0.56, -0.15] | 0.72 [0.31, 0.95] | 0.76 [0.47, 0.98] | 0.64 [ |
| 1.17 [0.91, 1.39] | | | | | | | |
| ypmr0 | SM8-Solvation | 0.50 [0.35, 0.63] | 0.44 [0.31, 0.58] | 0.07 [-0.22, 0.37] | 0.61 [0.26, 0.89] | 0.93 [0.53, 1.50] | 0.64 [ |
| 1.48 [1.46, 1.49] | | | | | | | |
| yd6ub | S+logP | 0.51 [0.32, 0.65] | 0.41 [0.22, 0.58] | 0.09 [-0.19, 0.38] | 0.63 [0.20, 0.90] | 0.99 [0.47, 1.41] | 0.53 [- |
| 0.73 [0.36, 1.08] | | | | | | | |
| 7egyc | SMD-Solvation-Trained | 0.52 [0.35, 0.66] | 0.44 [0.29, 0.61] | 0.27 [0.00, 0.54] | 0.57 [0.23, 0.84] | 0.50 [0.32, 0.76] | 0.45 [ |
| 1.45 [1.41, 1.48] | | | | | | | |
| 0a7a8 | ML Prediction using MD Feature Vector Trained ... | 0.53 [0.34, 0.69] | 0.43 [0.25, 0.62] | 0.32 [0.04, 0.56] | 0.62 [0.13, 0.90] | 0.74 [0.34, 1.02] | 0.45 [- |
| 1.01 [0.74, 1.26] | | | | | | | |
| 7dhtp | LogP-prediction-method-name | 0.54 [0.34, 0.71] | 0.44 [0.27, 0.64] | 0.06 [-0.27, 0.39] | 0.49 [0.07, 0.86] | 0.73 [0.26, 1.16] | 0.56 [ |
| 0.50 [0.19, 0.86] | | | | | | | |
| qyzjx | EC_RISM_dry_P1w+2o | 0.54 [0.34, 0.74] | 0.46 [0.31, 0.64] | -0.15 [-0.40, 0.20] | 0.73 [0.33, 0.97] | 1.22 [0.90, 1.47] | 0.78 [ |
| 1.22 [1.01, 1.36] | | | | | | | |
| w6jta | ML Prediction using MD Feature Vector Trained ... | 0.56 [0.34, 0.74] | 0.46 [0.28, 0.65] | 0.32 [0.07, 0.58] | 0.53 [0.12, 0.90] | 0.62 [0.36, 0.83] | 0.51 [ |
| 1.12 [0.85, 1.36] | | | | | | | |
| 5krdi | ZINC15 versus PM3 | 0.60 [0.39, 0.82] | 0.51 [0.32, 0.72] | -0.30 [-0.62, 0.00] | 0.63 [0.25, 0.91] | 1.03 [0.58, 1.50] | 0.60 [ |
| 0.37 [0.09, 0.66] | | | | | | | |
| ji2zm | SM8-Solvation-Trained | 0.60 [0.42, 0.75] | 0.53 [0.37, 0.69] | 0.45 [0.22, 0.67] | 0.66 [0.31, 0.89] | 0.66 [0.43, 0.99] | 0.51 [ |
| 1.43 [1.39, 1.47] | | | | | | | |
| gnxuu | ML Prediction using MD Feature Vector Trained ... | 0.61 [0.39, 0.80] | 0.51 [0.32, 0.73] | 0.40 [0.14, 0.67] | 0.53 [0.12, 0.92] | 0.57 [0.33, 0.77] | 0.51 [ |
| 1.10 [0.86, 1.31] | | | | | | | |
| tc4xa | NHLBI-NN-5HL | 0.62 [0.41, 0.80] | 0.51 [0.33, 0.73] | 0.17 [-0.19, 0.52] | 0.66 [0.15, 0.90] | 1.21 [0.53, 1.66] | 0.49 [- |
| 1.10 [0.86, 1.32] | | | | | | | |
| 6cdyo | SM12-Solvation | 0.65 [0.42, 0.83] | 0.54 [0.32, 0.75] | -0.24 [-0.62, 0.12] | 0.52 [0.19, 0.83] | 0.93 [0.49, 1.71] | 0.53 [ |
| 0.78 [0.47, 1.10] | | | | | | | |

Continued on next page

| ID | name | RMSE | MAE | ME | $R^2$ | m | ES |
|---|---|---|---|---|---|---|---|
| dbmg3 | GC-LSER | 0.70 [0.48, 0.90] | 0.60 [0.41, 0.82] | 0.42 [0.11, 0.77] | 0.47 [0.05, 0.81] | 0.75 [0.19, 1.33] | 0.38 [-1.43 [1.38, 1.47] |
| kxsp3 | PLS2 from NIST data and QM-generated QSAR Desc... | 0.74 [0.49, 0.96] | 0.62 [0.40, 0.87] | 0.48 [0.15, 0.80] | 0.36 [0.03, 0.76] | 0.54 [0.07, 1.10] | 0.35 [-0.71 [0.40, 1.03] |
| nh6c0 | Molecular-Dynamics-Expanded-Ensembles | 0.74 [0.56, 0.94] | 0.67 [0.49, 0.88] | 0.09 [-0.34, 0.55] | 0.62 [0.15, 0.87] | 1.34 [0.53, 1.93] | 0.49 [0.74 [0.49, 0.99] |
| kivfu | LogP-prediction-method-IEFPCM/MST | 0.78 [0.34, 1.09] | 0.56 [0.26, 0.90] | -0.03 [-0.54, 0.42] | 0.41 [0.03, 0.89] | 0.97 [0.23, 1.45] | 0.45 [-1.07 [0.74, 1.38] |
| ujsgv | Alchemical-CGenFF | 0.82 [0.53, 1.08] | 0.67 [0.37, 0.97] | -0.31 [-0.72, 0.17] | 0.33 [0.01, 0.84] | 0.80 [0.03, 1.47] | 0.35 [-1.27 [1.13, 1.40] |
| wu52s | LogP-PLS-ECFC4_CSsep-Bayer | 0.83 [0.57, 1.05] | 0.72 [0.49, 0.98] | 0.70 [0.42, 0.97] | 0.55 [0.09, 0.99] | 0.54 [0.24, 0.93] | 0.56 [-0.42 [0.17, 0.72] |
| 5mahv | ML Prediction using MD Feature Vector Trained ... | 0.85 [0.44, 1.16] | 0.62 [0.34, 0.98] | -0.02 [-0.53, 0.47] | 0.34 [0.02, 0.77] | 0.90 [0.21, 1.36] | 0.24 [-1.07 [0.77, 1.34] |
| g6dwz | NHLBI-NN-3HL | 0.85 [0.56, 1.07] | 0.72 [0.45, 0.97] | 0.35 [-0.11, 0.79] | 0.52 [0.09, 0.86] | 1.18 [0.51, 1.74] | 0.45 [-0.84 [0.53, 1.15] |
| bqeuh | ISIDA-LSER | 0.87 [0.52, 1.17] | 0.66 [0.35, 1.02] | 0.25 [-0.26, 0.77] | 0.01 [0.00, 0.52] | -0.05 [-0.42, 0.45] | 0.02 [-1.33 [1.19, 1.44] |
| d7vth | UFZ-LSER | 0.87 [0.62, 1.09] | 0.78 [0.56, 1.00] | -0.65 [-0.97, -0.33] | 0.63 [0.22, 0.94] | 1.11 [0.76, 1.38] | 0.49 [0.77 [0.53, 1.01] |
| 2mi5w | Alchemical-CGenFF | 0.95 [0.63, 1.24] | 0.81 [0.54, 1.12] | -0.30 [-0.84, 0.26] | 0.18 [0.00, 0.64] | 0.61 [-0.15, 1.27] | 0.24 [-1.21 [1.04, 1.35] |
| qz8d5 | SMD-Solvation | 0.97 [0.70, 1.19] | 0.84 [0.55, 1.13] | 0.77 [0.42, 1.11] | 0.53 [0.18, 0.84] | 0.93 [0.51, 1.55] | 0.48 [1.40 [1.34, 1.45] |
| kuddg | LogP-Pred-MTNN-GraphConv-Bayer | 0.97 [0.71, 1.19] | 0.89 [0.66, 1.12] | 0.89 [0.66, 1.12] | 0.67 [0.28, 0.95] | 0.71 [0.42, 1.04] | 0.53 [-0.17 [0.02, 0.34] |
| y0xxd | FS-GM (Fast switching Growth Method) | 1.04 [0.39, 1.50] | 0.72 [0.30, 1.21] | 0.37 [-0.16, 1.00] | 0.33 [0.00, 0.93] | 1.03 [-0.27, 2.01] | 0.42 [-1.31 [1.12, 1.47] |
| 2ggir | FS-AGM (Fast switching Annihilation/Growth Met... | 1.04 [0.82, 1.23] | 0.98 [0.74, 1.18] | -0.36 [-0.88, 0.28] | 0.31 [0.00, 0.93] | 0.98 [-0.29, 1.90] | 0.49 [0.83 [0.64, 1.02] |
| dyxbt | B3PW91-TZ SMD set1 | 1.07 [0.77, 1.36] | 0.96 [0.69, 1.25] | 0.96 [0.69, 1.25] | 0.55 [0.08, 0.92] | 0.68 [0.20, 1.16] | 0.56 [-0.00 [-0.00, -0.00] |
| mm0jf | LogP-prediction-SMD-HuangLab | 1.09 [0.93, 1.25] | 1.03 [0.82, 1.24] | 1.03 [0.82, 1.24] | 0.75 [0.39, 0.98] | 0.60 [0.38, 0.82] | 0.75 [1.09 [0.99, 1.22] |
| h83sb | Linear Regression with B3LYP/6-31G+ | 1.12 [0.59, 1.61] | 0.87 [0.48, 1.31] | -0.21 [-0.92, 0.40] | 0.00 [0.00, 0.58] | -0.02 [-1.03, 0.85] | -0.16 [0.33 [0.06, 0.58] |
| 3wvyh | Alchemical-CGenFF | 1.13 [0.50, 1.75] | 0.77 [0.35, 1.31] | 0.26 [-0.31, 1.06] | 0.37 [0.03, 0.93] | 1.24 [0.35, 2.26] | 0.55 [1.23 [0.94, 1.42] |
| f3dpg | PLS from NIST data and QM-generated QSAR Descr... | 1.17 [0.70, 1.56] | 0.92 [0.49, 1.39] | -0.85 [-1.36, -0.35] | 0.11 [0.00, 0.48] | 0.36 [-0.16, 0.81] | 0.15 [-0.63 [0.27, 1.00] |
| 25s67 | FS-AGM (Fast switching Annihilation/Growth Met... | 1.21 [0.83, 1.55] | 1.06 [0.71, 1.46] | -0.97 [-1.44, -0.53] | 0.63 [0.14, 0.90] | 1.33 [0.33, 2.34] | 0.45 [-0.79 [0.52, 1.06] |

Continued on next page

| ID | name | RMSE | MAE | ME | $R^2$ | m | |
|---|---|---|---|---|---|---|---|
| zdj0j | Solvation-B3LYP | 1.21 [0.97, 1.42] | 1.13 [0.86, 1.38] | 1.13 [0.86, 1.38] | 0.64 [0.25, 0.95] | 0.86 [0.39, 1.29] | 0.64 [ |
| 0.08 [-0.00, 0.32] | | | | | | | |
| 7gg6s | MLR from NIST data and QM-generated QSAR Descr... | 1.27 [0.84, 1.63] | 1.00 [0.58, 1.46] | -1.00 [-1.44, -0.57] | 0.10 [0.00, 0.46] | 0.31 [-0.12, 0.76] | 0.16 [- |
| 0.60 [0.22, 0.96] | | | | | | | |
| hwf2k | Extended solvent-contact model approach | 1.28 [0.55, 1.93] | 0.93 [0.47, 1.53] | -0.09 [-0.97, 0.58] | 0.12 [0.00, 0.85] | 0.68 [-0.85, 1.57] | 0.31 [- |
| 0.48 [0.23, 0.79] | | | | | | | |
| pcv32 | Solvation- WB97X-D | 1.28 [1.02, 1.54] | 1.17 [0.84, 1.49] | 1.17 [0.84, 1.49] | 0.50 [0.10, 0.90] | 0.75 [0.21, 1.40] | 0.44 [- |
| 0.28 [0.02, 0.50] | | | | | | | |
| v2q0t | InterX_GAFF_WET_OCTANOL | 1.31 [0.97, 1.66] | 1.16 [0.85, 1.53] | -1.15 [-1.52, -0.83] | 0.70 [0.27, 0.98] | 1.31 [0.92, 1.57] | 0.64 [ |
| 1.34 [1.25, 1.42] | | | | | | | |
| rdsnw | EC_RISM_wet_P1w+1o | 1.32 [0.85, 1.68] | 1.15 [0.78, 1.54] | 1.15 [0.78, 1.54] | 0.78 [0.43, 0.97] | 1.51 [1.13, 1.79] | 0.75 [ |
| 0.98 [0.71, 1.21] | | | | | | | |
| ggm6n | FS-GM (Fast switching Growth Method) | 1.32 [0.98, 1.64] | 1.16 [0.81, 1.53] | -1.15 [-1.53, -0.76] | 0.53 [0.11, 0.86] | 1.04 [0.39, 1.69] | 0.53 [ |
| 1.17 [1.00, 1.32] | | | | | | | |
| jjd0b | MD/S-MBIS-GAFF-TIP3P/MBAR/ | 1.35 [0.87, 1.78] | 1.13 [0.69, 1.63] | -1.09 [-1.60, -0.59] | 0.66 [0.22, 0.92] | 1.51 [0.80, 2.13] | 0.53 [ |
| 0.75 [0.47, 1.08] | | | | | | | |
| 2tzb0 | EC_RISM_dry_P1w+1o | 1.38 [0.94, 1.79] | 1.21 [0.84, 1.64] | 1.21 [0.84, 1.64] | 0.79 [0.40, 0.97] | 1.58 [1.23, 1.87] | 0.75 [ |
| 1.00 [0.76, 1.21] | | | | | | | |
| cr3hs | PLS3 from NIST data and QM-generated QSAR Desc... | 1.39 [0.58, 2.13] | 0.96 [0.47, 1.66] | 0.80 [0.23, 1.57] | 0.40 [0.01, 0.80] | 1.36 [-0.15, 2.68] | 0.35 [- |
| 0.65 [0.31, 1.01] | | | | | | | |
| arw58 | DLPNO-CCSD(T)/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.41 [0.81, 1.90] | 1.09 [0.61, 1.64] | 1.01 [0.46, 1.60] | 0.09 [0.00, 0.53] | -0.24 [-0.76, 0.25] | -0.20 [- |
| -0.00 [-0.00, -0.00] | | | | | | | |
| ahmtf | B3PW91-TZ SMD kcl-wet-oct | 1.41 [1.13, 1.70] | 1.33 [1.06, 1.63] | 1.33 [1.06, 1.63] | 0.55 [0.12, 0.89] | 0.70 [0.24, 1.14] | 0.56 [ |
| -0.00 [-0.00, -0.00] | | | | | | | |
| o7djk | B3PW91-TZ SMD wetoct | 1.42 [1.11, 1.73] | 1.34 [1.05, 1.65] | 1.34 [1.05, 1.65] | 0.55 [0.13, 0.89] | 0.70 [0.22, 1.20] | 0.56 [ |
| -0.00 [-0.00, -0.00] | | | | | | | |
| 4p2ph | DLPNO-Solv-ccCA | 1.44 [0.81, 1.96] | 1.12 [0.62, 1.72] | 1.04 [0.48, 1.70] | 0.09 [0.00, 0.54] | -0.26 [-0.78, 0.23] | -0.26 [- |
| -0.00 [-0.00, -0.00] | | | | | | | |
| fmf7r | dice | 1.44 [1.03, 1.77] | 1.25 [0.83, 1.67] | 0.26 [-0.63, 1.13] | 0.05 [0.00, 0.61] | 0.47 [-0.93, 2.15] | 0.10 [- |
| 0.32 [0.05, 0.67] | | | | | | | |
| 6fyg5 | Solvation-M062X | 1.50 [1.28, 1.70] | 1.44 [1.18, 1.67] | 1.44 [1.18, 1.67] | 0.69 [0.32, 0.96] | 0.93 [0.50, 1.52] | 0.71 [ |
| 0.05 [0.00, 0.18] | | | | | | | |
| sqosi | MD-AMBER-dryoct | 1.69 [1.12, 2.18] | 1.42 [0.86, 1.98] | -1.40 [-1.96, -0.82] | 0.51 [0.05, 0.89] | 1.40 [0.40, 2.05] | 0.45 [- |
| 0.72 [0.41, 1.05] | | | | | | | |
| rs4ns | BLYP/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.71 [1.07, 2.25] | 1.44 [0.89, 2.04] | 1.44 [0.89, 2.04] | 0.06 [0.00, 0.53] | -0.19 [-0.74, 0.28] | -0.22 [- |
| 0.07 [-0.00, 0.27] | | | | | | | |
| c7t5j | PBE/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.73 [1.15, 2.28] | 1.47 [0.96, 2.05] | 1.47 [0.96, 2.05] | 0.05 [0.00, 0.50] | -0.18 [-0.71, 0.31] | -0.16 [- |
| -0.00 [-0.00, 0.06] | | | | | | | |
| jc68f | PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.74 [1.15, 2.25] | 1.47 [0.95, 2.03] | 1.47 [0.95, 2.03] | 0.05 [0.00, 0.49] | -0.18 [-0.72, 0.28] | -0.16 [- |
| -0.00 [-0.00, 0.07] | | | | | | | |
| 03cyy | Linear Regression-B3LYP/6-311G** | 1.75 [0.62, 2.69] | 1.11 [0.45, 1.96] | 0.03 [-0.91, 1.10] | 0.00 [0.00, 0.52] | 0.12 [-1.13, 1.50] | 0.09 [- |
| 0.36 [0.07, 0.69] | | | | | | | |

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| ID<br>ES | name | RMSE | MAE | ME | $R^2$ | m | |
|---|---|---|---|---|---|---|---|
| hsotx<br>-0.00 [-0.00, 0.01] | B3LYP/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.81 [1.21, 2.33] | 1.56 [1.01, 2.11] | 1.56 [1.01, 2.11] | 0.07 [0.00, 0.49] | -0.19 [-0.63, 0.28] | -0.20 [ |
| ke5gu<br>0.49 [0.20, 0.78] | MD/S-MBIS-GAFF-SPCE/MBAR/ | 1.82 [1.29, 2.25] | 1.59 [1.03, 2.07] | -1.59 [-2.06, -1.03] | 0.62 [0.17, 0.89] | 1.54 [0.71, 2.21] | 0.53 [- |
| fe8ws<br>-0.00 [-0.00, -0.00] | B3PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.83 [1.28, 2.35] | 1.58 [1.10, 2.15] | 1.58 [1.10, 2.15] | 0.06 [0.00, 0.48] | -0.18 [-0.67, 0.25] | -0.16 [ |
| mwuua<br>0.49 [0.28, 0.73] | MD-LigParGen-wetoct | 1.83 [1.47, 2.11] | 1.73 [1.38, 2.06] | -1.73 [-2.06, -1.37] | 0.41 [0.01, 0.78] | 0.67 [0.03, 1.21] | 0.48 [- |
| fyx45<br>0.80 [0.47, 1.14] | LogP-prediction-Drude-FEP-HuangLab | 1.85 [0.66, 2.72] | 1.25 [0.55, 2.16] | 0.65 [-0.29, 1.78] | 0.63 [0.17, 0.92] | 2.63 [1.15, 3.87] | 0.67 [ |
| 5t0yn<br>-0.00 [-0.00, -0.00] | PBE0/cc-pVTZ//B3LYP-D3/cc-pVTZ | 1.85 [1.29, 2.39] | 1.61 [1.11, 2.15] | 1.61 [1.11, 2.15] | 0.06 [0.00, 0.49] | -0.18 [-0.62, 0.27] | -0.16 [ |
| 6nmtt<br>0.57 [0.35, 0.82] | MD-AMBER-wetoct | 1.87 [1.33, 2.45] | 1.65 [1.16, 2.19] | -1.65 [-2.17, -1.15] | 0.42 [0.04, 0.92] | 1.10 [0.34, 1.61] | 0.60 [ |
| eufcy<br>0.41 [0.22, 0.65] | MD-LigParGen-dryoct | 1.99 [1.60, 2.34] | 1.88 [1.48, 2.26] | -1.77 [-2.25, -1.18] | 0.54 [0.19, 0.87] | 1.43 [0.52, 2.38] | 0.66 [ |
| tzzb5<br>0.66 [0.36, 1.00] | Alchemical-CGenFF | 2.12 [1.57, 2.63] | 1.87 [1.28, 2.51] | 1.43 [0.56, 2.36] | 0.20 [0.00, 0.65] | -0.76 [-1.57, 0.20] | -0.20 [ |
| 3oqhx<br>0.75 [0.40, 1.13] | MD-CHARMM-dryoct | 2.14 [1.25, 2.86] | 1.64 [0.88, 2.48] | 1.11 [0.00, 2.25] | 0.03 [0.00, 0.44] | -0.44 [-1.85, 0.98] | 0.00 [- |
| bzeez<br>0.23 [0.06, 0.51] | FS-AGM (Fast switching Annihilation/Growth Met... | 2.20 [1.81, 2.51] | 2.07 [1.57, 2.47] | -2.07 [-2.47, -1.54] | 0.63 [0.19, 0.95] | 1.39 [0.85, 2.07] | 0.53 [ |
| 5svjv<br>0.74 [0.56, 0.96] | FS-GM (Fast switching Growth Method) | 2.26 [1.80, 2.67] | 2.14 [1.68, 2.60] | -2.03 [-2.59, -1.32] | 0.39 [0.02, 0.91] | 1.20 [0.35, 1.81] | 0.44 [- |
| ynquk<br>1.07 [0.95, 1.20] | TWOVAR | 2.26 [1.86, 2.60] | 2.13 [1.66, 2.56] | 2.13 [1.66, 2.56] | 0.08 [0.00, 0.77] | 0.25 [-0.29, 0.63] | 0.38 [- |
| odex0<br>1.09 [0.90, 1.30] | InterX_ARROW_2017_PIMD_SOLVENT2_WET_OCTANOL | 2.29 [1.63, 2.84] | 1.98 [1.30, 2.69] | 1.73 [0.84, 2.61] | 0.09 [0.00, 0.66] | -0.53 [-1.82, 0.78] | -0.09 [ |
| pnc4j<br>0.39 [0.17, 0.73] | LogP-prediction-Drude-Umbrella-HuangLab | 2.29 [1.64, 2.90] | 2.03 [1.38, 2.69] | 2.03 [1.38, 2.69] | 0.04 [0.00, 0.66] | 0.31 [-0.76, 1.27] | 0.20 [- |
| padym<br>1.09 [0.90, 1.27] | InterX_ARROW_2017_PIMD_WET_OCTANOL | 2.29 [1.65, 2.82] | 1.99 [1.33, 2.67] | 1.72 [0.77, 2.62] | 0.12 [0.00, 0.69] | -0.60 [-1.99, 0.76] | -0.13 [ |
| fcspk<br>1.06 [0.85, 1.26] | ARROW_2017_PIMD_SOLVENT2 | 2.40 [1.70, 2.98] | 2.10 [1.39, 2.82] | 1.97 [1.12, 2.79] | 0.11 [0.00, 0.64] | -0.50 [-1.56, 0.60] | -0.16 [ |
| 6cm6a<br>1.06 [0.86, 1.29] | ARROW_2017_PIMD | 2.41 [1.70, 2.94] | 2.10 [1.37, 2.82] | 1.94 [1.05, 2.79] | 0.19 [0.00, 0.69] | -0.66 [-1.78, 0.63] | -0.27 [ |
| bq6fo<br>0.23 [0.00, 0.42] | Extended solvent-contact model approach | 2.58 [1.67, 3.33] | 2.15 [1.33, 2.99] | 1.55 [0.31, 2.71] | 0.10 [0.00, 0.58] | 1.05 [-0.83, 2.57] | 0.09 [- |
| 4nfzz<br>0.20 [0.05, 0.38] | MD/S-HI-GAFF-TIP3P/MBAR/ | 2.67 [1.98, 3.35] | 2.44 [1.84, 3.14] | -2.44 [-3.13, -1.83] | 0.40 [0.05, 0.88] | 1.30 [0.54, 1.86] | 0.42 [- |
| 623c0<br>0.18 [0.09, 0.29] | MD-OPLSAA-wetoct | 2.67 [2.13, 3.28] | 2.53 [2.08, 3.12] | -2.53 [-3.10, -2.07] | 0.22 [0.01, 0.79] | 0.64 [-0.09, 1.13] | 0.38 [- |

Continued on next page

| ID | name | RMSE | MAE | ME | $R^2$ | m | |
|---|---|---|---|---|---|---|---|
| ES | | | | | | | |
| eg52i | ARROW_2017 | 2.86 [2.02, 3.53] | 2.41 [1.55, 3.28] | 2.06 [0.94, 3.17] | 0.15 [0.00, 0.60] | -0.94 [-2.43, 0.22] | -0.16 [ |
| 0.96 [0.70, 1.22] | | | | | | | |
| 5585v | Alchemical-CGenFF | 2.88 [1.97, 3.65] | 2.55 [1.78, 3.35] | 2.40 [1.38, 3.28] | 0.04 [0.00, 0.55] | -0.41 [-2.05, 0.72] | -0.20 [ |
| 0.46 [0.21, 0.73] | | | | | | | |
| cp8kv | MD-OPLSAA-dryoct | 2.88 [2.29, 3.60] | 2.72 [2.25, 3.35] | -2.72 [-3.34, -2.24] | 0.24 [0.00, 0.95] | 0.78 [-0.01, 1.42] | 0.59 [ |
| 0.12 [0.06, 0.21] | | | | | | | |
| j4nb3 | FOURVAR | 2.89 [2.35, 3.38] | 2.63 [1.89, 3.27] | 2.63 [1.89, 3.27] | 0.01 [0.00, 0.79] | 0.12 [-0.79, 0.91] | 0.16 [- |
| 0.89 [0.71, 1.08] | | | | | | | |
| hf4wj | MD/S-HI-GAFF-SPCE/MBAR/ | 3.28 [2.53, 4.11] | 3.04 [2.40, 3.85] | -3.04 [-3.83, -2.39] | 0.34 [0.03, 0.84] | 1.31 [0.40, 1.97] | 0.38 [- |
| 0.09 [0.02, 0.20] | | | | | | | |
| pku5g | SAMPL5_49_retro3 | 4.87 [4.06, 5.70] | 4.68 [3.89, 5.49] | 4.68 [3.89, 5.49] | 0.49 [0.02, 0.90] | 1.80 [0.27, 3.00] | 0.56 [- |
| 0.39 [0.25, 0.57] | | | | | | | |
| po4g2 | SAMPL5_49 | 5.46 [4.39, 6.61] | 5.17 [4.21, 6.28] | 5.17 [4.21, 6.28] | 0.51 [0.04, 0.87] | 2.33 [0.49, 3.74] | 0.56 [ |
| 0.34 [0.20, 0.52] | | | | | | | |

Notes
- RMSE: Root mean square error
- MAE: Mean absolute error
- ME: Mean error
- R2: R-squared, square of Pearson correlation coefficient
- m: slope of the line fit to predicted vs experimental logP values
- ES: error slope calculated from the QQ Plots of model uncertainty predictions
- Mean and 95% confidence intervals of RMSE, MAE, ME, R2, and m were calculated by bootstrapping with 10000 samples.
- 95% confidence intervals of ES were calculated by bootstrapping with 1000 samples.