ID	name	RMSE	MAE	ME	R^2	m
hmz0n	cosmotherm_FINE19	0.384 [0.225, 0.542]	0.309 [0.189, 0.450]	-0.167 [-0.357, 0.036]	0.767 [0.386, 0.942]	0.936 [0.640, 1.162]
gmoq5	Global XGBoost-Based QSPR LogP Predictor	0.392 [0.272, 0.485]	0.343 [0.231, 0.456]	0.012 [-0.207, 0.257]	0.741 [0.414, 0.929]	0.994 [0.688, 1.331]
3vqbi	cosmoquick_TZVP18+ML	0.409 [0.282, 0.528]	0.355 [0.236, 0.479]	-0.079 [-0.303, 0.185]	0.660 [0.233, 0.932]	0.784 [0.481, 1.079]
sq07q	Local XGBoost-Based QSPR LogP Predictor	0.465 [0.325, 0.577]	0.408 [0.269, 0.540]	0.028 [-0.254, 0.317]	0.640 [0.212, 0.892]	0.924 [0.516, 1.295]
j8nwc	EC_RISM_wet_P1w+2o	0.471 [0.163, 0.752]	0.310 [0.147, 0.547]	0.072 [-0.161, 0.400]	0.736 [0.302, 0.975]	1.142 [0.812, 1.398]
xxh4i	SM12-Solvation-Trained	0.490 [0.329, 0.622]	0.428 [0.292, 0.570]	0.185 [-0.106, 0.445]	0.543 [0.141, 0.882]	0.602 [0.285, 1.072]
hdpuj	RayLogP-II, a cheminformatic QSPR model predic...	0.492 [0.366, 0.613]	0.445 [0.327, 0.574]	-0.290 [-0.522, -0.032]	0.744 [0.352, 0.935]	1.016 [0.662, 1.366]
dqxk4	LogP_SMD_Solvation_DFT	0.495 [0.341, 0.618]	0.418 [0.269, 0.572]	0.302 [0.061, 0.521]	0.686 [0.364, 0.907]	0.833 [0.507, 1.228]
vzgyt	rfs-logp	0.496 [0.284, 0.683]	0.381 [0.217, 0.583]	-0.346 [-0.567, -0.149]	0.719 [0.310, 0.955]	0.761 [0.483, 0.948]
ypmr0	SM8-Solvation	0.499 [0.351, 0.627]	0.444 [0.316, 0.582]	0.075 [-0.235, 0.353]	0.614 [0.254, 0.879]	0.929 [0.526, 1.543]
yd6ub	S+logP	0.508 [0.337, 0.654]	0.405 [0.237, 0.588]	0.085 [-0.215, 0.401]	0.633 [0.204, 0.912]	0.986 [0.463, 1.407]
7egyc	SMD-Solvation-Trained	0.519 [0.345, 0.666]	0.442 [0.284, 0.605]	0.273 [-0.015, 0.517]	0.570 [0.205, 0.843]	0.505 [0.312, 0.775]
0a7a8	ML Prediction using MD Feature Vector Trained ...	0.528 [0.348, 0.688]	0.429 [0.259, 0.624]	0.316 [0.050, 0.565]	0.620 [0.104, 0.920]	0.738 [0.333, 1.008]
7dhtp	LogP-prediction-method-name	0.535 [0.339, 0.697]	0.436 [0.271, 0.615]	0.060 [-0.268, 0.358]	0.485 [0.116, 0.882]	0.728 [0.335, 1.147]
qyzjx	EC_RISM_dry_P1w+2o	0.536 [0.342, 0.748]	0.455 [0.306, 0.645]	-0.154 [-0.409, 0.182]	0.730 [0.325, 0.974]	1.216 [0.877, 1.478]
w6jta	ML Prediction using MD Feature Vector Trained ...	0.564 [0.309, 0.755]	0.457 [0.265, 0.665]	0.323 [0.066, 0.610]	0.533 [0.147, 0.902]	0.624 [0.384, 0.848]
ji2zm	SM8-Solvation-Trained	0.598 [0.428, 0.738]	0.533 [0.366, 0.685]	0.453 [0.215, 0.663]	0.656 [0.312, 0.899]	0.656 [0.418, 0.964]
5krdi	ZINC15 versus PM3	0.601 [0.400, 0.814]	0.508 [0.340, 0.710]	-0.301 [-0.590, 0.018]	0.635 [0.228, 0.913]	1.029 [0.581, 1.530]
gnxuu	ML Prediction using MD Feature Vector Trained ...	0.611 [0.382, 0.807]	0.505 [0.306, 0.725]	0.402 [0.125, 0.702]	0.527 [0.120, 0.924]	0.566 [0.332, 0.824]
tc4xa	NHLBI-NN-5HL	0.623 [0.408, 0.803]	0.515 [0.307, 0.728]	0.171 [-0.181, 0.525]	0.659 [0.160, 0.926]	1.213 [0.521, 1.684]
6cdyo	SM12-Solvation	0.646 [0.417, 0.838]	0.536 [0.319, 0.756]	-0.244 [-0.605, 0.107]	0.517 [0.220, 0.823]	0.927 [0.484, 1.660]
dbmg3	GC-LSER	0.697 [0.477, 0.900]	0.599 [0.400, 0.824]	0.425 [0.097, 0.752]	0.472 [0.043, 0.815]	0.746 [0.148, 1.275]
kxsp3	PLS2 from NIST data and QM-generated QSAR Desc...	0.739 [0.489, 0.946]	0.623 [0.392, 0.867]	0.477 [0.133, 0.802]	0.365 [0.017, 0.728]	0.537 [0.049, 1.109]
nh6c0	Molecular-Dynamics-Expanded-Ensembles	0.745 [0.561, 0.937]	0.671 [0.496, 0.865]	0.087 [-0.362, 0.547]	0.617 [0.152, 0.884]	1.341 [0.529, 1.925]
kivfu	LogP-prediction-method-IEFPCM/MST	0.779 [0.297, 1.094]	0.563 [0.245, 0.916]	-0.032 [-0.520, 0.409]	0.407 [0.030, 0.919]	0.967 [0.332, 1.467]
ujsgv	Alchemical-CGenFF	0.821 [0.551, 1.070]	0.670 [0.388, 0.965]	-0.310 [-0.731, 0.165]	0.335 [0.005, 0.824]	0.797 [-0.014, 1.455]
wu52s	LogP-PLS-ECFC4_CSsep-Bayer	0.828 [0.594, 1.061]	0.723 [0.503, 0.981]	0.697 [0.445, 0.973]	0.550 [0.123, 0.987]	0.537 [0.244, 0.876]
g6dwz	NHLBI-NN-3HL	0.847 [0.561, 1.079]	0.715 [0.446, 0.988]	0.346 [-0.144, 0.835]	0.516 [0.057, 0.853]	1.183 [0.414, 1.720]
5mahv	ML Prediction using MD Feature Vector Trained ...	0.849 [0.450, 1.178]	0.625 [0.325, 0.981]	-0.015 [-0.527, 0.509]	0.336 [0.036, 0.768]	0.903 [0.352, 1.339]
bqeuh	ISIDA-LSER	0.866 [0.495, 1.178]	0.657 [0.326, 1.012]	0.248 [-0.255, 0.756]	0.006 [0.000, 0.529]	-0.051 [-0.449, 0.445]
d7vth	UFZ-LSER	0.867 [0.615, 1.104]	0.778 [0.551, 1.026]	-0.653 [-0.967, -0.287]	0.628 [0.201, 0.945]	1.106 [0.716, 1.357]
2mi5w	Alchemical-CGenFF	0.946 [0.649, 1.257]	0.813 [0.551, 1.131]	-0.300 [-0.822, 0.233]	0.182 [0.002, 0.657]	0.606 [-0.210, 1.238]
kuddg	LogP-Pred-MTNN-GraphConv-Bayer	0.966 [0.707, 1.199]	0.887 [0.665, 1.128]	0.887 [0.665, 1.128]	0.672 [0.231, 0.950]	0.712 [0.420, 1.083]
qz8d5	SMD-Solvation	0.972 [0.705, 1.193]	0.844 [0.555, 1.135]	0.773 [0.406, 1.119]	0.527 [0.131, 0.838]	0.930 [0.459, 1.521]
y0xxd	FS-GM (Fast switching Growth Method)	1.041 [0.469, 1.515]	0.719 [0.307, 1.203]	0.366 [-0.132, 0.989]	0.331 [0.003, 0.929]	1.028 [-0.161, 2.020]
2ggir	FS-AGM (Fast switching Annihilation/Growth Met...	1.042 [0.838, 1.244]	0.976 [0.756, 1.195]	-0.356 [-0.885, 0.248]	0.307 [0.002, 0.921]	0.977 [-0.351, 1.860]
dyxbt	B3PW91-TZ SMD set1	1.065 [0.786, 1.356]	0.958 [0.696, 1.247]	0.958 [0.696, 1.247]	0.546 [0.090, 0.898]	0.682 [0.188, 1.143]
mm0jf	LogP-prediction-SMD-HuangLab	1.089 [0.915, 1.238]	1.031 [0.815, 1.220]	1.031 [0.815, 1.220]	0.751 [0.403, 0.979]	0.602 [0.386, 0.825]
h83sb	Linear Regression with B3LYP/6-31G+	1.117 [0.566, 1.600]	0.869 [0.466, 1.336]	-0.209 [-0.937, 0.417]	0.000 [0.000, 0.593]	-0.019 [-1.132, 0.901]
3wvyh	Alchemical-CGenFF	1.132 [0.480, 1.779]	0.766 [0.346, 1.384]	0.265 [-0.344, 1.028]	0.366 [0.018, 0.940]	1.241 [0.297, 2.202]
f3dpg	PLS from NIST data and QM-generated QSAR Descr...	1.173 [0.730, 1.532]	0.922 [0.493, 1.347]	-0.851 [-1.318, -0.363]	0.110 [0.002, 0.476]	0.362 [-0.142, 0.865]
25s67	FS-AGM (Fast switching Annihilation/Growth Met...	1.211 [0.827, 1.526]	1.057 [0.692, 1.415]	-0.974 [-1.379, -0.523]	0.626 [0.139, 0.900]	1.332 [0.364, 2.376]
zdj0j	Solvation-B3LYP	1.215 [0.971, 1.426]	1.133 [0.847, 1.389]	1.133 [0.847, 1.389]	0.640 [0.238, 0.950]	0.856 [0.401, 1.297]

Continued on next page

ID	name	RMSE	MAE	ME	R^2	m
7gg6s	MLR from NIST data and QM-generated QSAR Descr...	1.266 [0.820, 1.631]	1.005 [0.552, 1.476]	-1.005 [-1.473, -0.548]	0.101 [0.001, 0.455]	0.312 [-0.247, 0.764]
hwf2k	Extended solvent-contact model approach	1.276 [0.560, 1.852]	0.934 [0.485, 1.455]	-0.094 [-0.909, 0.561]	0.116 [0.001, 0.858]	0.682 [-0.632, 1.612]
pcv32	Solvation- WB97X-D	1.284 [1.028, 1.529]	1.170 [0.854, 1.471]	1.170 [0.854, 1.471]	0.498 [0.114, 0.894]	0.750 [0.251, 1.418]
v2q0t	InterX_GAFF_WET_OCTANOL	1.305 [0.938, 1.638]	1.165 [0.811, 1.497]	-1.154 [-1.495, -0.766]	0.698 [0.232, 0.981]	1.310 [0.927, 1.565]
rdsnw	EC_RISM_wet_P1w+1o	1.315 [0.861, 1.723]	1.151 [0.798, 1.555]	1.151 [0.798, 1.555]	0.777 [0.399, 0.964]	1.509 [1.122, 1.797]
ggm6n	FS-GM (Fast switching Growth Method)	1.323 [0.934, 1.642]	1.164 [0.765, 1.538]	-1.151 [-1.532, -0.726]	0.533 [0.130, 0.839]	1.042 [0.459, 1.766]
jjd0b	MD/S-MBIS-GAFF-TIP3P/MBAR/	1.351 [0.908, 1.743]	1.135 [0.718, 1.597]	-1.095 [-1.574, -0.614]	0.663 [0.246, 0.904]	1.505 [0.814, 2.069]
2tzb0	EC_RISM_dry_P1w+1o	1.380 [0.937, 1.784]	1.209 [0.842, 1.605]	1.209 [0.842, 1.605]	0.790 [0.396, 0.972]	1.578 [1.202, 1.865]
cr3hs	PLS3 from NIST data and QM-generated QSAR Desc...	1.386 [0.590, 2.137]	0.961 [0.468, 1.648]	0.805 [0.217, 1.585]	0.403 [0.009, 0.788]	1.361 [-0.269, 2.649]
arw58	DLPNO-CCSD(T)/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.406 [0.873, 1.909]	1.094 [0.624, 1.648]	1.010 [0.481, 1.613]	0.087 [0.000, 0.604]	-0.242 [-0.744, 0.267]
ahmtf	B3PW91-TZ SMD kcl-wet-oct	1.413 [1.129, 1.711]	1.334 [1.065, 1.637]	1.334 [1.065, 1.637]	0.550 [0.097, 0.896]	0.699 [0.235, 1.189]
o7djk	B3PW91-TZ SMD wetoct	1.417 [1.153, 1.692]	1.338 [1.084, 1.625]	1.338 [1.084, 1.625]	0.550 [0.125, 0.897]	0.698 [0.254, 1.170]
fmf7r	dice	1.438 [1.019, 1.789]	1.251 [0.837, 1.689]	0.264 [-0.635, 1.105]	0.049 [0.000, 0.604]	0.465 [-0.888, 2.064]
4p2ph	DLPNO-Solv-ccCA	1.440 [0.894, 1.959]	1.120 [0.636, 1.725]	1.042 [0.510, 1.678]	0.095 [0.000, 0.601]	-0.259 [-0.801, 0.249]
6fyg5	Solvation-M062X	1.497 [1.294, 1.712]	1.438 [1.204, 1.692]	1.438 [1.204, 1.692]	0.691 [0.331, 0.960]	0.929 [0.508, 1.539]
sqosi	MD-AMBER-dryoct	1.692 [1.117, 2.169]	1.417 [0.872, 1.976]	-1.403 [-1.953, -0.832]	0.515 [0.048, 0.872]	1.403 [0.407, 2.034]
rs4ns	BLYP/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.714 [1.131, 2.278]	1.438 [0.911, 2.021]	1.438 [0.911, 2.021]	0.064 [0.000, 0.521]	-0.192 [-0.741, 0.262]
c7t5j	PBE/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.733 [1.150, 2.241]	1.465 [0.955, 2.040]	1.465 [0.955, 2.040]	0.054 [0.000, 0.495]	-0.176 [-0.698, 0.290]
jc68f	PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.735 [1.137, 2.274]	1.469 [0.922, 2.045]	1.469 [0.922, 2.045]	0.054 [0.000, 0.495]	-0.175 [-0.720, 0.311]
03cyy	Linear Regression-B3LYP/6-311G**	1.755 [0.536, 2.882]	1.107 [0.411, 2.125]	0.029 [-0.856, 1.278]	0.002 [0.000, 0.561]	0.121 [-1.254, 1.450]
hsotx	B3LYP/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.809 [1.240, 2.350]	1.557 [1.047, 2.141]	1.557 [1.047, 2.141]	0.069 [0.000, 0.498]	-0.190 [-0.741, 0.268]
ke5gu	MD/S-MBIS-GAFF-SPCE/MBAR/	1.818 [1.279, 2.304]	1.594 [1.064, 2.144]	-1.594 [-2.135, -1.045]	0.622 [0.166, 0.896]	1.537 [0.701, 2.186]
mwuua	MD-LigParGen-wetoct	1.826 [1.497, 2.129]	1.731 [1.405, 2.081]	-1.731 [-2.078, -1.402]	0.406 [0.015, 0.764]	0.670 [0.113, 1.151]
fe8ws	B3PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.828 [1.222, 2.341]	1.585 [1.068, 2.137]	1.585 [1.068, 2.137]	0.060 [0.000, 0.492]	-0.176 [-0.673, 0.271]
5t0yn	PBE0/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.848 [1.247, 2.393]	1.607 [1.069, 2.181]	1.607 [1.069, 2.181]	0.059 [0.000, 0.499]	-0.176 [-0.641, 0.268]
fyx45	LogP-prediction-Drude-FEP-HuangLab	1.855 [0.654, 2.797]	1.254 [0.522, 2.226]	0.654 [-0.256, 1.866]	0.628 [0.160, 0.917]	2.634 [1.071, 3.848]
6nmtt	MD-AMBER-wetoct	1.867 [1.345, 2.486]	1.653 [1.192, 2.260]	-1.653 [-2.250, -1.191]	0.417 [0.017, 0.920]	1.100 [0.158, 1.570]
eufcy	MD-LigParGen-dryoct	1.989 [1.630, 2.329]	1.880 [1.502, 2.261]	-1.765 [-2.255, -1.191]	0.543 [0.175, 0.878]	1.425 [0.507, 2.387]
tzzb5	Alchemical-CGenFF	2.119 [1.512, 2.580]	1.866 [1.251, 2.474]	1.434 [0.450, 2.341]	0.195 [0.003, 0.604]	-0.760 [-1.556, 0.286]
3oqhx	MD-CHARMM-dryoct	2.143 [1.219, 2.895]	1.642 [0.888, 2.508]	1.105 [0.060, 2.218]	0.033 [0.000, 0.390]	-0.435 [-1.882, 0.973]
bzeez	FS-AGM (Fast switching Annihilation/Growth Met...	2.202 [1.821, 2.534]	2.068 [1.556, 2.495]	-2.068 [-2.491, -1.554]	0.631 [0.149, 0.953]	1.389 [0.815, 2.096]
ynquk	TWOVAR	2.259 [1.850, 2.580]	2.130 [1.645, 2.536]	2.130 [1.645, 2.536]	0.079 [0.000, 0.755]	0.246 [-0.273, 0.632]
5svjv	FS-GM (Fast switching Growth Method)	2.265 [1.835, 2.682]	2.141 [1.719, 2.576]	-2.028 [-2.565, -1.404]	0.389 [0.036, 0.913]	1.195 [0.434, 1.747]
odex0	InterX_ARROW_2017_PIMD_SOLVENT2_WET_OCTANOL	2.288 [1.599, 2.810]	1.980 [1.284, 2.631]	1.731 [0.738, 2.569]	0.093 [0.000, 0.640]	-0.528 [-1.758, 0.755]
padym	InterX_ARROW_2017_PIMD_WET_OCTANOL	2.288 [1.664, 2.837]	1.986 [1.319, 2.679]	1.717 [0.769, 2.615]	0.124 [0.000, 0.699]	-0.604 [-1.900, 0.695]
pnc4j	LogP-prediction-Drude-Umbrella-HuangLab	2.290 [1.669, 2.883]	2.033 [1.436, 2.672]	2.033 [1.436, 2.672]	0.045 [0.000, 0.639]	0.308 [-0.890, 1.333]
fcspk	ARROW_2017_PIMD_SOLVENT2	2.402 [1.671, 2.936]	2.100 [1.363, 2.759]	1.969 [1.068, 2.736]	0.112 [0.000, 0.654]	-0.502 [-1.578, 0.640]
6cm6a	ARROW_2017_PIMD	2.411 [1.786, 2.952]	2.105 [1.454, 2.790]	1.937 [1.043, 2.779]	0.189 [0.001, 0.696]	-0.662 [-1.766, 0.464]
bq6fo	Extended solvent-contact model approach	2.577 [1.687, 3.348]	2.155 [1.355, 3.023]	1.555 [0.366, 2.671]	0.104 [0.000, 0.605]	1.049 [-1.002, 2.660]
623c0	MD-OPLSAA-wetoct	2.665 [2.158, 3.235]	2.533 [2.104, 3.065]	-2.533 [-3.055, -2.101]	0.224 [0.003, 0.810]	0.641 [-0.065, 1.099]
4nfzz	MD/S-HI-GAFF-TIP3P/MBAR/	2.667 [1.979, 3.384]	2.436 [1.837, 3.154]	-2.436 [-3.142, -1.828]	0.397 [0.029, 0.890]	1.298 [0.472, 1.895]
eg52i	ARROW_2017	2.862 [2.022, 3.495]	2.411 [1.518, 3.277]	2.062 [0.940, 3.186]	0.147 [0.002, 0.580]	-0.938 [-2.193, 0.274]
cp8kv	MD-OPLSAA-dryoct	2.877 [2.325, 3.585]	2.721 [2.285, 3.322]	-2.721 [-3.311, -2.282]	0.239 [0.005, 0.930]	0.777 [0.096, 1.431]

Continued on next page

ID	name	RMSE	MAE	ME	R^2	m
5585v	Alchemical-CGenFF	2.881 [2.002, 3.656]	2.555 [1.783, 3.352]	2.400 [1.428, 3.302]	0.043 [0.000, 0.574]	-0.408 [-1.926, 0.659]
j4nb3	FOURVAR	2.890 [2.325, 3.332]	2.629 [1.839, 3.237]	2.629 [1.839, 3.237]	0.006 [0.000, 0.797]	0.122 [-0.831, 0.888]
hf4wj	MD/S-HI-GAFF-SPCE/MBAR/	3.284 [2.502, 4.153]	3.037 [2.341, 3.879]	-3.037 [-3.873, -2.334]	0.336 [0.023, 0.860]	1.313 [0.404, 1.995]
pku5g	SAMPL5_49_retro3	4.868 [4.055, 5.737]	4.680 [3.901, 5.541]	4.680 [3.901, 5.541]	0.487 [0.041, 0.912]	1.797 [0.309, 3.137]
po4g2	SAMPL5_49	5.461 [4.433, 6.694]	5.166 [4.234, 6.311]	5.166 [4.234, 6.311]	0.506 [0.030, 0.897]	2.326 [0.273, 3.834]

Notes

- Mean and 95% confidence intervals of statistic values were calculated by bootstrapping.