

ID	name	RMSE		MAE		ME		R <sup>2</sup>		m		$\tau$		ES	
hmz0n	cosmotherm_FINE19	0.38	[0.23, 0.55]	0.31	[0.20, 0.45]	-0.17	[-0.37, 0.02]	0.77	[0.37, 0.94]	0.94	[0.61, 1.18]	0.64	[0.17, 1.00]	1.15	[0.93, 1.33]
gmoq5	Global XGBoost-Based QSPR LogP Predictor	0.39	[0.28, 0.49]	0.34	[0.22, 0.46]	0.01	[-0.21, 0.25]	0.74	[0.43, 0.92]	0.99	[0.70, 1.34]	0.59	[0.15, 0.91]	0.69	[0.42, 1.00]
3vqbi	cosmoquick_TZVP18+ML	0.41	[0.29, 0.53]	0.36	[0.24, 0.48]	-0.08	[-0.31, 0.18]	0.66	[0.26, 0.93]	0.78	[0.51, 1.11]	0.56	[0.12, 0.91]	1.06	[0.85, 1.26]
j8nwc	EC-RISM_wet_P1w+2o	0.47	[0.17, 0.75]	0.31	[0.15, 0.55]	0.07	[-0.16, 0.40]	0.74	[0.33, 0.97]	1.14	[0.85, 1.41]	0.81	[0.40, 1.00]	1.31	[1.08, 1.46]
sq07q	Local XGBoost-Based QSPR LogP Predictor	0.47	[0.34, 0.58]	0.41	[0.28, 0.54]	0.03	[-0.22, 0.29]	0.64	[0.21, 0.88]	0.92	[0.53, 1.29]	0.56	[0.12, 0.88]	0.60	[0.30, 0.95]
xxh4i	SM12-Solvation-Trained	0.49	[0.33, 0.62]	0.43	[0.29, 0.57]	0.18	[-0.11, 0.43]	0.54	[0.16, 0.86]	0.60	[0.31, 1.00]	0.51	[0.02, 0.88]	1.41	[1.36, 1.46]
dqkx4	LogP_SMD_Solvation_DFT	0.49	[0.34, 0.63]	0.42	[0.26, 0.59]	0.30	[0.08, 0.55]	0.69	[0.35, 0.92]	0.83	[0.51, 1.26]	0.67	[0.27, 0.96]	1.13	[0.92, 1.33]
hdpuj	RayLogP-II, a cheminformatic QSPR model predic...	0.49	[0.37, 0.61]	0.44	[0.32, 0.58]	-0.29	[-0.52, -0.04]	0.74	[0.39, 0.94]	1.02	[0.69, 1.37]	0.67	[0.18, 1.00]	0.91	[0.69, 1.12]
vzgyt	rfs-logp	0.50	[0.27, 0.68]	0.38	[0.21, 0.58]	-0.35	[-0.56, -0.14]	0.72	[0.32, 0.95]	0.76	[0.48, 1.00]	0.64	[0.28, 0.95]	1.17	[0.92, 1.38]
ypmr0	SM8-Solvation	0.50	[0.35, 0.63]	0.44	[0.31, 0.59]	0.07	[-0.24, 0.36]	0.61	[0.24, 0.89]	0.93	[0.51, 1.48]	0.64	[0.25, 0.92]	1.48	[1.46, 1.49]
yd6ub	S+logP	0.51	[0.32, 0.65]	0.41	[0.23, 0.58]	0.09	[-0.20, 0.38]	0.63	[0.20, 0.89]	0.99	[0.49, 1.41]	0.53	[0.02, 0.87]	0.73	[0.37, 1.09]
7egyc	SMD-Solvation-Trained	0.52	[0.34, 0.67]	0.44	[0.28, 0.61]	0.27	[0.02, 0.55]	0.57	[0.21, 0.86]	0.50	[0.32, 0.80]	0.45	[0.02, 0.84]	1.45	[1.41, 1.48]
0a7a8	ML Prediction using MD Feature Vector Trained ...	0.53	[0.34, 0.69]	0.43	[0.25, 0.61]	0.32	[0.03, 0.56]	0.62	[0.15, 0.92]	0.74	[0.33, 1.03]	0.45	[-0.16, 0.87]	1.01	[0.75, 1.27]
7dhtp	LogP-prediction-method-name	0.54	[0.32, 0.71]	0.44	[0.25, 0.63]	0.06	[-0.27, 0.35]	0.49	[0.04, 0.89]	0.73	[0.23, 1.14]	0.56	[0.00, 0.96]	0.50	[0.18, 0.86]
qyzjx	EC_RISM_dry_P1w+2o	0.54	[0.34, 0.75]	0.46	[0.30, 0.65]	-0.15	[-0.41, 0.19]	0.73	[0.31, 0.97]	1.22	[0.90, 1.49]	0.78	[0.47, 1.00]	1.22	[1.01, 1.36]
w6jta	ML Prediction using MD Feature Vector Trained ...	0.56	[0.33, 0.75]	0.46	[0.28, 0.66]	0.32	[0.05, 0.60]	0.53	[0.15, 0.90]	0.62	[0.37, 0.84]	0.51	[0.04, 0.87]	1.12	[0.86, 1.34]
5krdi	ZINC15 versus PM3	0.60	[0.40, 0.82]	0.51	[0.33, 0.73]	-0.30	[-0.61, 0.02]	0.63	[0.22, 0.90]	1.03	[0.59, 1.49]	0.60	[0.13, 0.96]	0.37	[0.10, 0.67]
ji2zm	SM8-Solvation-Trained	0.60	[0.43, 0.75]	0.53	[0.38, 0.71]	0.45	[0.20, 0.68]	0.66	[0.30, 0.91]	0.66	[0.43, 1.00]	0.51	[0.12, 0.84]	1.43	[1.39, 1.47]
gnxuu	ML Prediction using MD Feature Vector Trained ...	0.61	[0.38, 0.80]	0.51	[0.31, 0.71]	0.40	[0.15, 0.66]	0.53	[0.12, 0.91]	0.57	[0.28, 0.79]	0.51	[0.04, 0.88]	1.10	[0.86, 1.32]
tc4xa	NHLBI-NN-5HL	0.62	[0.40, 0.81]	0.51	[0.32, 0.73]	0.17	[-0.21, 0.54]	0.66	[0.13, 0.91]	1.21	[0.41, 1.67]	0.49	[-0.06, 0.88]	1.10	[0.88, 1.32]
6cdyo	SM12-Solvation	0.65	[0.43, 0.83]	0.54	[0.34, 0.76]	-0.24	[-0.59, 0.12]	0.52	[0.20, 0.84]	0.93	[0.49, 1.78]	0.53	[0.17, 0.88]	0.78	[0.45, 1.11]
dbmg3	GC-LSER	0.70	[0.48, 0.90]	0.60	[0.41, 0.81]	0.42	[0.09, 0.75]	0.47	[0.02, 0.79]	0.75	[0.13, 1.28]	0.38	[-0.22, 0.83]	1.43	[1.38, 1.47]
kxsp3	PLS2 from NIST data and QM-generated QSAR Desc...	0.74	[0.50, 0.94]	0.62	[0.40, 0.86]	0.48	[0.15, 0.80]	0.36	[0.03, 0.74]	0.54	[0.06, 1.17]	0.35	[-0.22, 0.80]	0.71	[0.38, 1.03]
nh6c0	Molecular-Dynamics-Expanded-Ensembles	0.74	[0.55, 0.94]	0.67	[0.48, 0.87]	0.09	[-0.34, 0.56]	0.62	[0.19, 0.89]	1.34	[0.62, 1.96]	0.49	[0.02, 0.91]	0.74	[0.52, 0.98]
kivfu	LogP-prediction-method-IEFPCM/MST	0.78	[0.33, 1.08]	0.56	[0.27, 0.91]	-0.03	[-0.50, 0.44]	0.41	[0.03, 0.91]	0.97	[0.23, 1.46]	0.45	[-0.02, 0.84]	1.07	[0.73, 1.35]
ujsgv	Alchemical-CGenFF	0.82	[0.55, 1.08]	0.67	[0.39, 0.97]	-0.31	[-0.75, 0.15]	0.33	[0.01, 0.82]	0.80	[-0.01, 1.48]	0.35	[-0.13, 0.79]	1.27	[1.13, 1.38]
wu52s	LogP-PLS-ECFC4_CSsep-Bayer	0.83	[0.57, 1.05]	0.72	[0.49, 0.97]	0.70	[0.42, 0.96]	0.55	[0.09, 0.99]	0.54	[0.21, 0.85]	0.56	[-0.06, 1.00]	0.42	[0.16, 0.75]
5mahv	ML Prediction using MD Feature Vector Trained ...	0.85	[0.39, 1.19]	0.62	[0.30, 0.99]	-0.02	[-0.53, 0.48]	0.34	[0.03, 0.82]	0.90	[0.19, 1.39]	0.24	[-0.36, 0.75]	1.07	[0.77, 1.34]
g6dwz	NHLBI-NN-3HL	0.85	[0.56, 1.09]	0.72	[0.45, 1.00]	0.35	[-0.10, 0.82]	0.52	[0.07, 0.85]	1.18	[0.46, 1.73]	0.45	[-0.04, 0.87]	0.84	[0.51, 1.15]
bqeuu	ISIDA-LSER	0.87	[0.48, 1.16]	0.66	[0.33, 1.01]	0.25	[-0.22, 0.74]	0.01	[0.00, 0.58]	-0.05	[-0.44, 0.53]	0.02	[-0.53, 0.57]	1.33	[1.19, 1.43]
d7vth	UFZ-LSER	0.87	[0.61, 1.10]	0.78	[0.56, 1.01]	-0.65	[-0.97, -0.30]	0.63	[0.21, 0.92]	1.11	[0.70, 1.37]	0.49	[0.04, 0.84]	0.77	[0.53, 1.01]
2mi5w	Alchemical-CGenFF	0.95	[0.64, 1.23]	0.81	[0.55, 1.11]	-0.30	[-0.83, 0.22]	0.18	[0.00, 0.63]	0.61	[-0.07, 1.24]	0.24	[-0.18, 0.68]	1.21	[1.03, 1.35]
qz8d5	SMD-Solvation	0.97	[0.69, 1.19]	0.84	[0.54, 1.12]	0.77	[0.40, 1.11]	0.53	[0.18, 0.85]	0.93	[0.47, 1.58]	0.48	[0.08, 0.83]	1.40	[1.34, 1.45]
kuddg	LogP-Pred-MTNN-GraphConv-Bayer	0.97	[0.74, 1.18]	0.89	[0.68, 1.10]	0.89	[0.68, 1.10]	0.67	[0.25, 0.94]	0.71	[0.42, 1.03]	0.53	[-0.06, 0.92]	1.17	[0.93, 1.36]
y0xxd	FS-GM (Fast switching Growth Method)	1.04	[0.39, 1.48]	0.72	[0.30, 1.20]	0.37	[-0.15, 0.95]	0.33	[0.00, 0.94]	1.03	[-0.11, 2.00]	0.42	[-0.12, 0.92]	1.31	[1.12, 1.45]
2eggr	FS-AGM (Fast switching Annihilation/Growth Met...	1.04	[0.83, 1.24]	0.98	[0.75, 1.18]	-0.36	[-0.92, 0.26]	0.31	[0.00, 0.93]	0.98	[-0.27, 1.91]	0.49	[-0.02, 0.92]	0.83	[0.65, 1.03]
dyxbt	B3PW91-TZ SMD set1	1.07	[0.79, 1.35]	0.96	[0.71, 1.25]	0.96	[0.71, 1.25]	0.55	[0.10, 0.90]	0.68	[0.21, 1.16]	0.56	[0.11, 0.92]	-0.00	[-0.00, -0.00]
mm0jf	LogP-prediction-SMD-HuangLab	1.09	[0.91, 1.24]	1.03	[0.80, 1.22]	1.03	[0.80, 1.22]	0.75	[0.44, 0.98]	0.60	[0.39, 0.82]	0.75	[0.35, 1.00]	1.09	[0.98, 1.21]
h83sb	Linear Regression with B3LYP/6-31G+	1.12	[0.57, 1.61]	0.87	[0.48, 1.34]	-0.21	[-0.89, 0.36]	0.00	[0.00, 0.58]	-0.02	[-1.09, 0.87]	-0.16	[-0.67, 0.46]	0.33	[0.06, 0.57]
3wvvy	Alchemical-CGenFF	1.13	[0.51, 1.74]	0.77	[0.35, 1.33]	0.26	[-0.33, 0.98]	0.37	[0.02, 0.94]	1.24	[0.27, 2.29]	0.55	[0.09, 0.96]	1.23	[0.97, 1.42]
f3dpg	PLS from NIST data and QM-generated QSAR Descr...	1.17	[0.77, 1.53]	0.92	[0.52, 1.36]	-0.85	[-1.33, -0.37]	0.11	[0.00, 0.48]	0.36	[-0.26, 0.83]	0.15	[-0.36, 0.51]	0.63	[0.27, 1.03]
25s67	FS-AGM (Fast switching Annihilation/Growth Met...	1.21	[0.85, 1.56]	1.06	[0.71, 1.43]	-0.97	[-1.39, -0.53]	0.63	[0.12, 0.90]	1.33	[0.31, 2.39]	0.45	[-0.10, 0.88]	0.79	[0.51, 1.08]
zjd0j	Solvation-B3LYP	1.21	[0.99, 1.41]	1.13	[0.86, 1.37]	1.13	[0.86, 1.37]	0.64	[0.23, 0.95]	0.86	[0.41, 1.28]	0.64	[0.16, 0.96]	0.08	[0.00, 0.33]
7gg6s	MLR from NIST data and QM-generated QSAR Descr...	1.27	[0.84, 1.62]	1.00	[0.58, 1.46]	-1.00	[-1.45, -0.57]	0.10	[0.00, 0.51]	0.31	[-0.22, 0.75]	0.16	[-0.33, 0.56]	0.60	[0.24, 1.01]
hwf2k	Extended solvent-contact model approach	1.28	[0.55, 1.99]	0.93	[0.48, 1.57]	-0.09	[-0.99, 0.55]	0.12	[0.00, 0.84]	0.68	[-0.60, 1.70]	0.31	[-0.31, 0.83]	0.48	[0.23, 0.80]
pcv32	Solvation- WB97X-D	1.28	[1.01, 1.53]	1.17	[0.85, 1.47]	1.17	[0.85, 1.47]	0.50	[0.11, 0.90]	0.75	[0.24, 1.40]	0.44	[-0.10, 0.79]	0.28	[0.02, 0.50]
v2q0t	InterX_GAFF_WET_OCTANOL	1.31	[0.97, 1.66]	1.16	[0.85, 1.52]	-1.15	[-1.51, -0.81]	0.70	[0.24, 0.98]	1.31	[0.88, 1.57]	0.64	[0.17, 0.96]	1.34	[1.26, 1.42]
rdnsnw	EC_RISM_wet_P1w+1o	1.32	[0.86, 1.71]	1.15	[0.79, 1.55]	1.15	[0.79, 1.55]	0.78	[0.39, 0.97]	1.51	[1.16, 1.76]	0.75	[0.36, 1.00]	0.98	[0.75, 1.22]
ggm6n	FS-GM (Fast switching Growth Method)	1.32	[0.96, 1.65]	1.16	[0.79, 1.55]	-1.15	[-1.54, -0.74]	0.53	[0.10, 0.84]	1.04	[0.48, 1.68]	0.53	[0.06, 0.87]	1.17	[1.02, 1.32]
jjd0b	MD/S-MBIS-GAFF-TIP3P/MBAR/	1.35	[0.88, 1.72]	1.13	[0.73, 1.58]	-1.09	[-1.56, -0.63]	0.66	[0.21, 0.91]	1.51	[0.80, 2.07]	0.53	[0.02, 0.91]	0.75	[0.47, 1.07]
2tzb0	EC_RISM_dry_P1w+1o	1.38	[0.90, 1.81]	1.21	[0.82, 1.65]	1.21	[0.82, 1.65]	0.79	[0.43, 0.97]	1.58	[1.19, 1.84]	0.75	[0.36, 1.00]	1.00	[0.77, 1.21]
cr3hs	PLS3 from NIST data and QM-generated QSAR Desc...	1.39	[0.59, 2.15]	0.96	[0.47, 1.67]	0.80	[0.22, 1.55]	0.40	[0.01, 0.81]	1.36	[-0.28, 2.86]	0.35	[-0.35, 0.80]	0.65	[0.33, 0.96]
arw58	DLPNO-CCSD(T)/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.41	[0.79, 1.90]	1.09	[0.60, 1.65]	1.01	[0.45, 1.62]	0.09	[0.00, 0.56]	-0.24	[-0.83, 0.30]	-0.20	[-0.64, 0.39]	-0.00	[-0.00, -0.00]
ahmtf	B3PW91-TZ SMD kcl-wet-oct	1.41	[1.13, 1.71]	1.33	[1.07, 1.62]	1.33	[1.07, 1.62]	0.55	[0.12, 0.91]	0.70	[0.21, 1.16]	0.56	[0.13, 0.92]	-0.00	[-0.00, -0.00]
o7djk	B3PW91-TZ SMD wetoct	1.42	[1.15, 1.70]	1.34	[1.09, 1.61]	1.34	[1.09, 1.61]	0.55	[0.13, 0.89]	0.70	[0.24, 1.20]	0.56	[0.11, 0.92]	-0.00	[-0.00, -0.00]
4p2ph	DLPNO-Solv-ccCA	1.44	[0.82, 1.96]	1.12	[0.61, 1.69]	1.04	[0.45, 1.66]	0.09	[0.00, 0.58]	-0.26	[-0.77, 0.21]	-0.26	[-0.72, 0.25]	-0.00	[-0.00, 0.01]
fmf7r	dice	1.44	[0.99, 1.77]	1.25	[0.79, 1.66]	0.26	[-0.60, 1.12]	0.05	[0.00, 0.60]	0.47	[-0.96, 2.02]	0.10	[-0.56, 0.65]	0.32	[0.05, 0.68]
6fyg5	Solvation-M062X	1.50	[1.26, 1.72]	1.44	[1.18, 1.67]	1.44	[1.18, 1.67]	0.69	[0.33, 0.97]	0.93	[0.49, 1.52]	0.71	[0.28, 1.00]	0.05	[0.00, 0.17]
sqosi	MD-AMBER-dryoct	1.69	[1.10, 2.16]	1.42	[0.87, 1.95]	-1.40	[-1.94, -0.81]	0.51	[0.04, 0.88]	1.40	[0.33, 2.06]	0.45	[-0.02, 0.87]	0.72	[0.43, 1.02]
rs4ns	BLYP/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.71	[1.12, 2.26]	1.44	[0.90, 2.01]	1.44	[0.90, 2.01]	0.06	[0.00, 0.50]	-0.19	[-0.71, 0.32]	-0.22	[-0.71, 0.33]	0.07	[-0.00, 0.26]
c7t5j	PBE/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.73	[1.10, 2.23]	1.47	[0.90, 1.99]	1.47	[0.90, 1.99]	0.05	[0.00, 0.50]	-0.18	[-0.70, 0.33]	-0.16	[-0.62, 0.46]	-0.00	[-0.00, 0.06]
jc68f	PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.74	[1.16, 2.27]	1.47	[0.95, 2.06]	1.47	[0.95, 2.06]	0.05	[0.00, 0.49]	-0.18					

ID	name	RMSE		MAE		ME		R <sup>2</sup>		m		$\tau$		ES	
fe8ws	B3PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.83	[1.25, 2.34]	1.58	[1.08, 2.13]	1.58	[1.08, 2.13]	0.06	[0.00, 0.50]	-0.18	[-0.70, 0.26]	-0.16	[-0.62, 0.38]	-0.00	[-0.00, -0.00]
mwuuua	MD-LigParGen-wetoct	1.83	[1.48, 2.13]	1.73	[1.37, 2.07]	-1.73	[-2.07, -1.36]	0.41	[0.01, 0.78]	0.67	[0.07, 1.16]	0.48	[-0.03, 0.87]	0.49	[0.29, 0.72]
fyx45	LogP-prediction-Drude-FEP-HuangLab	1.85	[0.61, 2.69]	1.25	[0.51, 2.10]	0.65	[-0.34, 1.66]	0.63	[0.17, 0.92]	2.63	[1.02, 3.84]	0.67	[0.16, 1.00]	0.80	[0.45, 1.12]
5t0yn	PBE0/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.85	[1.27, 2.35]	1.61	[1.09, 2.15]	1.61	[1.09, 2.15]	0.06	[0.00, 0.48]	-0.18	[-0.68, 0.26]	-0.16	[-0.64, 0.45]	-0.00	[-0.00, -0.00]
6nmmt	MD-AMBER-wetoct	1.87	[1.35, 2.49]	1.65	[1.18, 2.24]	-1.65	[-2.24, -1.17]	0.42	[0.02, 0.91]	1.10	[0.21, 1.54]	0.60	[0.08, 1.00]	0.57	[0.34, 0.83]
eufcy	MD-LigParGen-dryoct	1.99	[1.61, 2.36]	1.88	[1.47, 2.29]	-1.77	[-2.29, -1.18]	0.54	[0.14, 0.89]	1.43	[0.46, 2.39]	0.66	[0.17, 1.00]	0.41	[0.22, 0.66]
tzzb5	Alchemical-CGenFF	2.12	[1.51, 2.60]	1.87	[1.23, 2.49]	1.43	[0.53, 2.37]	0.20	[0.00, 0.60]	-0.76	[-1.68, 0.31]	-0.20	[-0.61, 0.33]	0.66	[0.37, 0.99]
3oqhxx	MD-CHARMM-dryoct	2.14	[1.20, 2.91]	1.64	[0.82, 2.50]	1.11	[0.04, 2.20]	0.03	[0.00, 0.46]	-0.44	[-2.06, 1.16]	0.00	[-0.52, 0.53]	0.75	[0.38, 1.13]
bzeez	FS-AGM (Fast switching Annihilation/Growth Met...	2.20	[1.86, 2.50]	2.07	[1.59, 2.46]	-2.07	[-2.46, -1.58]	0.63	[0.19, 0.96]	1.39	[0.88, 2.10]	0.53	[0.04, 0.92]	0.23	[0.06, 0.50]
5svjv	FS-GM (Fast switching Growth Method)	2.26	[1.82, 2.70]	2.14	[1.69, 2.60]	-2.03	[-2.57, -1.35]	0.39	[0.05, 0.90]	1.20	[0.51, 1.75]	0.44	[-0.12, 0.91]	0.74	[0.55, 0.94]
ynquk	TWOVAR	2.26	[1.86, 2.59]	2.13	[1.66, 2.55]	2.13	[1.66, 2.55]	0.08	[0.00, 0.75]	0.25	[-0.23, 0.63]	0.38	[-0.10, 0.80]	1.07	[0.95, 1.21]
padym	InterX_ARROW_2017_PIMD_WET_OCTANOL	2.29	[1.62, 2.83]	1.99	[1.31, 2.66]	1.72	[0.81, 2.60]	0.12	[0.00, 0.70]	-0.60	[-1.94, 0.86]	-0.13	[-0.67, 0.48]	1.09	[0.90, 1.29]
odex0	InterX_ARROW_2017_PIMD_SOLVENT2_WET_OCTANOL	2.29	[1.63, 2.84]	1.98	[1.29, 2.66]	1.73	[0.85, 2.56]	0.09	[0.00, 0.67]	-0.53	[-1.77, 0.82]	-0.09	[-0.60, 0.47]	1.09	[0.90, 1.27]
pnc4j	LogP-prediction-Drude-Umbrella-HuangLab	2.29	[1.64, 2.88]	2.03	[1.38, 2.72]	2.03	[1.38, 2.72]	0.04	[0.00, 0.62]	0.31	[-0.86, 1.25]	0.20	[-0.40, 0.69]	0.39	[0.16, 0.72]
fcspk	ARROW_2017_PIMD_SOLVENT2	2.40	[1.76, 2.93]	2.10	[1.43, 2.76]	1.97	[1.17, 2.74]	0.11	[0.00, 0.59]	-0.50	[-1.58, 0.51]	-0.16	[-0.63, 0.40]	1.06	[0.87, 1.27]
6cm6a	ARROW_2017_PIMD	2.41	[1.79, 2.96]	2.10	[1.41, 2.84]	1.94	[1.10, 2.76]	0.19	[0.00, 0.65]	-0.66	[-1.67, 0.44]	-0.27	[-0.71, 0.33]	1.06	[0.87, 1.27]
bq6fo	Extended solvent-contact model approach	2.58	[1.65, 3.32]	2.15	[1.33, 3.02]	1.55	[0.36, 2.72]	0.10	[0.00, 0.61]	1.05	[-1.07, 2.67]	0.09	[-0.40, 0.59]	0.23	[0.01, 0.40]
4nfzz	MD/S-HI-GAFF-TIP3P/MBAR/	2.67	[1.97, 3.35]	2.44	[1.82, 3.12]	-2.44	[-3.11, -1.81]	0.40	[0.02, 0.90]	1.30	[0.42, 1.94]	0.42	[-0.16, 0.87]	0.20	[0.05, 0.38]
623c0	MD-OPLSAA-wetoct	2.67	[2.15, 3.25]	2.53	[2.10, 3.09]	-2.53	[-3.07, -2.09]	0.22	[0.00, 0.81]	0.64	[-0.09, 1.11]	0.38	[-0.10, 0.84]	0.18	[0.09, 0.29]
eg52i	ARROW_2017	2.86	[2.00, 3.57]	2.41	[1.50, 3.36]	2.06	[0.86, 3.26]	0.15	[0.00, 0.53]	-0.94	[-2.09, 0.42]	-0.16	[-0.59, 0.38]	0.96	[0.70, 1.21]
5585v	Alchemical-CGenFF	2.88	[1.98, 3.72]	2.55	[1.80, 3.41]	2.40	[1.41, 3.35]	0.04	[0.00, 0.60]	-0.41	[-1.88, 0.56]	-0.20	[-0.80, 0.30]	0.46	[0.21, 0.72]
cp8kv	MD-OPLSAA-dryoct	2.88	[2.32, 3.61]	2.72	[2.28, 3.37]	-2.72	[-3.35, -2.27]	0.24	[0.00, 0.92]	0.78	[0.02, 1.59]	0.59	[0.11, 1.00]	0.12	[0.06, 0.21]
j4nb3	FOURVAR	2.89	[2.30, 3.35]	2.63	[1.83, 3.26]	2.63	[1.83, 3.26]	0.01	[0.00, 0.77]	0.12	[-0.67, 0.95]	0.16	[-0.38, 0.80]	0.89	[0.72, 1.12]
hf4wj	MD/S-HI-GAFF-SPCE/MBAR/	3.28	[2.45, 4.12]	3.04	[2.31, 3.85]	-3.04	[-3.84, -2.31]	0.34	[0.03, 0.87]	1.31	[0.45, 2.02]	0.38	[-0.15, 0.88]	0.09	[0.01, 0.20]
pku5g	SAMPL5_49_retro3	4.87	[4.08, 5.74]	4.68	[3.92, 5.58]	4.68	[3.92, 5.58]	0.49	[0.04, 0.92]	1.80	[0.27, 3.06]	0.56	[-0.02, 0.96]	0.39	[0.24, 0.58]
po4g2	SAMPL5_49	5.46	[4.38, 6.59]	5.17	[4.23, 6.26]	5.17	[4.23, 6.26]	0.51	[0.06, 0.90]	2.33	[0.57, 3.76]	0.56	[0.04, 1.00]	0.34	[0.19, 0.53]

## 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
- $\tau$ : Kendall rank correlation coefficient
- 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.