

ID	name	RMSE		MAE		ME		R <sup>2</sup>		m		$\tau$		ES	
hmq0n	cosmothrm_FINE19	0.38	[0.23, 0.54]	0.31	[0.19, 0.45]	-0.17	[-0.37, 0.01]	0.77	[0.40, 0.94]	0.94	[0.61, 1.16]	0.64	[0.20, 1.00]	1.15	[0.93, 1.33]
gmoq5	Global XGBoost-Based QSPR LogP Predictor	0.39	[0.27, 0.49]	0.34	[0.23, 0.47]	0.01	[-0.21, 0.27]	0.74	[0.33, 0.92]	0.99	[0.66, 1.36]	0.59	[0.04, 0.88]	0.69	[0.38, 1.00]
3vqbi	cosmoquick_TZVP18+ML	0.41	[0.28, 0.53]	0.36	[0.23, 0.48]	-0.08	[-0.29, 0.20]	0.66	[0.30, 0.93]	0.78	[0.53, 1.15]	0.56	[0.13, 0.91]	1.06	[0.84, 1.25]
j8nwc	EC_RISM_wet_P1w+2o	0.47	[0.17, 0.75]	0.31	[0.15, 0.55]	0.07	[-0.15, 0.39]	0.74	[0.34, 0.97]	1.14	[0.85, 1.38]	0.81	[0.46, 1.00]	1.31	[1.07, 1.46]
sq07q	Local XGBoost-Based QSPR LogP Predictor	0.47	[0.34, 0.58]	0.41	[0.28, 0.54]	0.03	[-0.25, 0.28]	0.64	[0.23, 0.88]	0.92	[0.53, 1.28]	0.56	[0.06, 0.88]	0.60	[0.32, 0.91]
xxh4i	SM12-Solvation-Trained	0.49	[0.33, 0.62]	0.43	[0.29, 0.57]	0.18	[-0.11, 0.42]	0.54	[0.17, 0.87]	0.60	[0.30, 1.00]	0.51	[0.02, 0.91]	1.41	[1.36, 1.46]
dqk4i	LogP-SMD_Solvation_DFT	0.49	[0.34, 0.62]	0.42	[0.26, 0.58]	0.30	[0.05, 0.53]	0.69	[0.39, 0.91]	0.83	[0.48, 1.26]	0.67	[0.21, 0.96]	1.13	[0.94, 1.33]
hdpuj	RayLogP-II, a cheminformatic QSPR model predic...	0.49	[0.37, 0.61]	0.44	[0.32, 0.58]	-0.29	[-0.53, -0.04]	0.74	[0.36, 0.94]	1.02	[0.68, 1.35]	0.67	[0.22, 1.00]	0.91	[0.70, 1.12]
vzgyt	rfs-logp	0.50	[0.26, 0.70]	0.38	[0.20, 0.59]	-0.35	[-0.57, -0.13]	0.72	[0.28, 0.96]	0.76	[0.48, 1.00]	0.64	[0.25, 0.96]	1.17	[0.93, 1.39]
ypmr0	SM8-Solvation	0.50	[0.37, 0.63]	0.44	[0.32, 0.59]	0.07	[-0.21, 0.37]	0.61	[0.29, 0.89]	0.93	[0.54, 1.52]	0.64	[0.21, 0.92]	1.48	[1.46, 1.49]
yd6ub	S+logP	0.51	[0.32, 0.66]	0.41	[0.23, 0.60]	0.09	[-0.19, 0.39]	0.63	[0.20, 0.89]	0.99	[0.49, 1.41]	0.53	[-0.02, 0.88]	0.73	[0.39, 1.08]
7egyc	SMD-Solvation-Trained	0.52	[0.36, 0.67]	0.44	[0.28, 0.61]	0.27	[-0.00, 0.51]	0.57	[0.22, 0.85]	0.50	[0.32, 0.77]	0.45	[0.04, 0.80]	1.45	[1.41, 1.48]
0a7a8	ML Prediction using MD Feature Vector Trained ...	0.53	[0.34, 0.68]	0.43	[0.25, 0.61]	0.32	[0.06, 0.57]	0.62	[0.11, 0.90]	0.74	[0.34, 1.02]	0.45	[-0.18, 0.84]	1.01	[0.73, 1.26]
REF11	logP(o/w) (MOE)	0.54	[0.25, 0.81]	0.39	[0.19, 0.63]	0.19	[-0.09, 0.50]	0.59	[0.36, 0.89]	0.90	[0.34, 1.68]	0.67	[0.32, 0.96]	0.07	[-0.00, 0.32]
7dhtp	LogP-prediction-method-name	0.54	[0.33, 0.71]	0.44	[0.26, 0.63]	0.06	[-0.29, 0.36]	0.49	[0.06, 0.88]	0.73	[0.26, 1.17]	0.56	[0.04, 0.96]	0.50	[0.16, 0.86]
qyzjx	EC_RISM_dry_P1w+2o	0.54	[0.34, 0.74]	0.46	[0.31, 0.64]	-0.15	[-0.41, 0.19]	0.73	[0.35, 0.97]	1.22	[0.91, 1.48]	0.78	[0.43, 1.00]	1.22	[1.01, 1.37]
REF13	SlogP (MOE)	0.55	[0.37, 0.72]	0.47	[0.31, 0.65]	-0.27	[-0.55, 0.01]	0.69	[0.29, 0.92]	1.06	[0.53, 1.58]	0.60	[0.10, 0.96]	0.01	[-0.00, 0.16]
w6jta	ML Prediction using MD Feature Vector Trained ...	0.56	[0.32, 0.76]	0.46	[0.27, 0.67]	0.32	[0.05, 0.60]	0.53	[0.14, 0.90]	0.62	[0.35, 0.85]	0.51	[0.02, 0.91]	1.12	[0.85, 1.34]
REF10	hLogP (MOE)	0.60	[0.37, 0.83]	0.43	[0.32, 0.72]	-0.04	[-0.43, 0.30]	0.38	[0.01, 0.82]	0.65	[-0.07, 1.26]	0.35	[-0.25, 0.80]	0.02	[-0.00, 0.13]
5krdi	ZINC15 versus PM3	0.60	[0.39, 0.81]	0.51	[0.33, 0.70]	-0.30	[-0.64, 0.01]	0.63	[0.29, 0.91]	1.03	[0.59, 1.50]	0.60	[0.20, 0.92]	0.37	[0.08, 0.67]
REF12	MoKa_logP	0.60	[0.40, 0.76]	0.52	[0.35, 0.69]	-0.08	[-0.45, 0.27]	0.67	[0.22, 0.91]	1.21	[0.78, 1.57]	0.55	[0.04, 0.91]	-0.00	[-0.00, 0.01]
ji2zm	SM8-Solvation-Trained	0.60	[0.43, 0.74]	0.53	[0.37, 0.70]	0.45	[0.20, 0.68]	0.66	[0.34, 0.90]	0.66	[0.44, 0.98]	0.51	[0.13, 0.87]	1.43	[1.39, 1.47]
gnxuu	ML Prediction using MD Feature Vector Trained ...	0.61	[0.39, 0.81]	0.51	[0.31, 0.73]	0.40	[0.14, 0.69]	0.53	[0.15, 0.91]	0.57	[0.35, 0.80]	0.51	[0.04, 0.88]	1.10	[0.88, 1.31]
tc4xa	NHLBI-NN-5HL	0.62	[0.42, 0.80]	0.51	[0.32, 0.72]	0.17	[-0.18, 0.56]	0.66	[0.19, 0.92]	1.21	[0.60, 1.72]	0.49	[0.00, 0.84]	1.10	[0.87, 1.32]
6cdyo	SM12-Solvation	0.65	[0.44, 0.83]	0.54	[0.34, 0.75]	-0.24	[-0.61, 0.10]	0.52	[0.16, 0.82]	0.93	[0.41, 1.71]	0.53	[0.11, 0.84]	0.78	[0.47, 1.09]
dbmg3	GC-LSER	0.70	[0.48, 0.90]	0.60	[0.40, 0.82]	0.42	[0.09, 0.75]	0.47	[0.04, 0.80]	0.75	[0.12, 1.27]	0.38	[-0.16, 0.80]	1.43	[1.38, 1.47]
kxsp3	PLS2 from NIST data and QM-generated QSAR Desc...	0.74	[0.50, 0.95]	0.62	[0.39, 0.87]	0.48	[0.15, 0.82]	0.36	[0.01, 0.79]	0.54	[0.00, 1.22]	0.35	[-0.21, 0.83]	0.71	[0.38, 1.04]
nh6c0	Molecular-Dynamics-Expanded-Ensembles	0.74	[0.55, 0.94]	0.67	[0.47, 0.88]	0.09	[-0.36, 0.57]	0.62	[0.12, 0.88]	1.34	[0.52, 1.92]	0.49	[0.04, 0.91]	0.74	[0.51, 0.97]
kivfu	LogP-prediction-method-IEFPCM/MST	0.78	[0.36, 1.09]	0.56	[0.27, 0.90]	-0.03	[-0.53, 0.42]	0.41	[0.02, 0.87]	0.97	[0.20, 1.40]	0.45	[-0.06, 0.81]	1.07	[0.71, 1.35]
NULL0	mean clogP of FDA approved oral drugs (1998-2017)	0.79	[0.51, 1.03]	0.66	[0.43, 0.93]	0.42	[0.03, 0.83]	0.00	[0.00, 0.00]	0.00	[0.00, 0.00]	nan	[nan, nan]	-0.00	[-0.00, 0.13]
REF09	clogP (Biobyte)	0.82	[0.52, 1.09]	0.68	[0.42, 0.96]	-0.26	[-0.70, 0.24]	0.46	[0.08, 0.90]	1.09	[0.43, 1.84]	0.48	[0.00, 0.88]	0.01	[-0.00, 0.17]
ujsgv	Alchemical-CGenFF	0.82	[0.56, 1.05]	0.67	[0.40, 0.95]	-0.31	[-0.75, 0.17]	0.33	[0.01, 0.81]	0.80	[-0.01, 1.41]	0.35	[-0.13, 0.79]	1.27	[1.14, 1.39]
wu52s	LogP-PLS-ECFC4_CSsep-Bayer	0.83	[0.58, 1.06]	0.72	[0.50, 0.98]	0.70	[0.43, 0.97]	0.55	[0.14, 0.98]	0.54	[0.27, 0.89]	0.56	[-0.02, 1.00]	0.42	[0.15, 0.76]
5mahv	ML Prediction using MD Feature Vector Trained ...	0.85	[0.44, 1.19]	0.62	[0.32, 0.98]	-0.02	[-0.54, 0.46]	0.34	[0.02, 0.77]	0.90	[0.19, 1.45]	0.24	[-0.29, 0.74]	1.07	[0.77, 1.33]
g6dwz	NHLBI-NN-3HL	0.85	[0.56, 1.09]	0.72	[0.44, 1.01]	0.35	[-0.10, 0.81]	0.52	[0.09, 0.86]	1.18	[0.53, 1.69]	0.45	[-0.06, 0.87]	0.84	[0.54, 1.16]
bqeuu	ISIDA-LSER	0.87	[0.51, 1.17]	0.66	[0.33, 1.00]	0.25	[-0.23, 0.74]	0.01	[0.00, 0.51]	-0.05	[-0.43, 0.48]	0.02	[-0.57, 0.60]	1.33	[1.19, 1.44]
d7vth	UFZ-LSER	0.87	[0.62, 1.10]	0.78	[0.56, 1.02]	-0.65	[-0.99, -0.30]	0.63	[0.19, 0.95]	1.11	[0.67, 1.39]	0.49	[-0.02, 0.88]	0.77	[0.54, 1.04]
2mi5w	Alchemical-CGenFF	0.95	[0.63, 1.24]	0.81	[0.52, 1.12]	-0.30	[-0.83, 0.27]	0.18	[0.00, 0.66]	0.61	[-0.12, 1.25]	0.24	[-0.23, 0.69]	1.21	[1.04, 1.36]
qz8d5	SMD-Solvation	0.97	[0.71, 1.19]	0.84	[0.55, 1.13]	0.77	[0.41, 1.11]	0.53	[0.18, 0.84]	0.93	[0.47, 1.60]	0.48	[0.06, 0.82]	1.40	[1.34, 1.45]
kuddg	LogP-Pred-MTNN-GraphConv-Bayer	0.97	[0.72, 1.19]	0.89	[0.67, 1.12]	0.89	[0.67, 1.12]	0.67	[0.26, 0.95]	0.71	[0.43, 1.04]	0.53	[-0.06, 0.96]	0.17	[0.04, 0.35]
y0xxd	FS-GM (Fast switching Growth Method)	1.04	[0.38, 1.48]	0.72	[0.29, 1.18]	0.37	[-0.16, 0.96]	0.33	[0.00, 0.93]	1.03	[-0.19, 1.99]	0.42	[-0.12, 0.91]	1.31	[1.10, 1.47]
2ggir	FS-AGM (Fast switching Annihilation/Growth Met...	1.04	[0.84, 1.23]	0.98	[0.76, 1.19]	-0.36	[-0.91, 0.25]	0.31	[0.00, 0.92]	0.98	[-0.40, 1.88]	0.49	[0.00, 0.92]	0.83	[0.65, 1.03]
dyxbt	B3PW91-TZ SMD set1	1.07	[0.77, 1.35]	0.96	[0.68, 1.24]	0.96	[0.68, 1.24]	0.55	[0.07, 0.90]	0.68	[0.17, 1.16]	0.56	[0.09, 0.91]	-0.00	[-0.00, -0.00]
mm0jf	LogP-prediction-SMD-HuangLab	1.09	[0.90, 1.24]	1.03	[0.80, 1.21]	1.03	[0.80, 1.21]	0.75	[0.43, 0.98]	0.60	[0.37, 0.82]	0.75	[0.33, 1.00]	1.09	[0.99, 1.21]
h83sb	Linear Regression with B3LYP/6-31G+	1.12	[0.57, 1.55]	0.87	[0.48, 1.31]	-0.21	[-0.90, 0.41]	0.00	[0.00, 0.58]	-0.02	[-1.06, 0.86]	-0.16	[-0.73, 0.42]	0.33	[0.06, 0.60]
3wvyh	Alchemical-CGenFF	1.13	[0.48, 1.71]	0.77	[0.35, 1.28]	0.26	[-0.32, 0.92]	0.37	[0.04, 0.92]	1.24	[0.35, 2.24]	0.55	[0.06, 0.96]	1.23	[0.97, 1.42]
f3dpg	PLS from NIST data and QM-generated QSAR Descr...	1.17	[0.74, 1.54]	0.92	[0.50, 1.40]	-0.85	[-1.38, -0.38]	0.11	[0.00, 0.45]	0.36	[-0.10, 0.90]	0.15	[-0.32, 0.54]	0.63	[0.26, 1.02]
25s67	FS-AGM (Fast switching Annihilation/Growth Met...	1.21	[0.85, 1.55]	1.06	[0.72, 1.42]	-0.97	[-1.39, -0.54]	0.63	[0.23, 0.91]	1.33	[0.61, 2.35]	0.45	[-0.11, 0.88]	0.79	[0.52, 1.05]
zdj0j	Solvation-B3LYP	1.21	[0.99, 1.42]	1.13	[0.87, 1.39]	1.13	[0.87, 1.39]	0.64	[0.25, 0.94]	0.86	[0.41, 1.31]	0.64	[0.14, 0.96]	0.08	[-0.00, 0.31]
7gg6s	MLR from NIST data and QM-generated QSAR Descr...	1.27	[0.80, 1.64]	1.00	[0.54, 1.51]	-1.00	[-1.50, -0.53]	0.10	[0.00, 0.46]	0.31	[-0.14, 0.76]	0.16	[-0.36, 0.55]	0.60	[0.23, 1.01]
hwf2k	Extended solvent-contact model approach	1.28	[0.57, 1.94]	0.93	[0.48, 1.54]	-0.09	[-0.98, 0.61]	0.12	[0.00, 0.88]	0.68	[-0.64, 1.59]	0.31	[-0.33, 0.77]	0.48	[0.24, 0.81]
pcv32	Solvation- WB97X-D	1.28	[0.99, 1.53]	1.17	[0.85, 1.47]	1.17	[0.85, 1.47]	0.50	[0.12, 0.88]	0.75	[0.25, 1.40]	0.44	[-0.12, 0.81]	0.28	[0.02, 0.49]
v2q0t	InterX_GAFF_WET_OCTANOL	1.31	[0.94, 1.68]	1.16	[0.81, 1.56]	-1.15	[-1.56, -0.78]	0.70	[0.26, 0.98]	1.31	[0.91, 1.63]	0.64	[0.14, 0.96]	1.34	[1.25, 1.42]
rdsnw	EC_RISM_wet_P1w+1o	1.32	[0.87, 1.72]	1.15	[0.81, 1.54]	1.15	[0.81, 1.54]	0.78	[0.42, 0.97]	1.51	[1.14, 1.75]	0.75	[0.38, 1.00]	0.98	[0.73, 1.20]
ggm6n	FS-GM (Fast switching Growth Method)	1.32	[0.97, 1.64]	1.16	[0.80, 1.54]	-1.15	[-1.53, -0.75]	0.53	[0.10, 0.83]	1.04	[0.44, 1.65]	0.53	[0.04, 0.87]	1.17	[1.01, 1.32]
jjd0b	MD/S-MBIS-GAFF-TIP3P/MBAR/	1.35	[0.90, 1.76]	1.13	[0.74, 1.58]	-1.09	[-1.55, -0.63]	0.66	[0.24, 0.91]	1.51	[0.84, 2.02]	0.53	[-0.02, 0.91]	0.75	[0.44, 1.05]
2tzbo	EC_RISM_dry_P1w+1o	1.38	[0.94, 1.81]	1.21	[0.84, 1.63]	1.21	[0.84, 1.63]	0.79	[0.43, 0.97]	1.58	[1.21, 1.88]	0.75	[0.35, 1.00]	1.00	[0.76, 1.22]
cr3hs	PLS3 from NIST data and QM-generated QSAR Desc...	1.39	[0.58, 2.10]	0.96	[0.47, 1.61]	0.80	[0.21, 1.54]	0.40	[0.01, 0.79]	1.36	[-0.26, 2.71]	0.35	[-0.33, 0.84]	0.65	[0.32, 0.99]
arw58	DLPNO-CCSD(T)/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.41	[0.88, 1.91]	1.09	[0.62, 1.65]	1.01	[0.46, 1.62]	0.09	[0.00, 0.55]	-0.24	[-0.70, 0.25]	-0.20	[-0.63, 0.30]	-0.00	[-0.00, -0.00]
ahmtf	B3PW91-TZ SMD kcl-wet-oct	1.41	[1.13, 1.69]	1.33	[1.07, 1.62]	1.33	[1.07, 1.62]	0.55	[0.11, 0.90]	0.70	[0.25, 1.17]	0.56	[0.14, 0.92]	-0.00	[-0.00, -0.00]
o7djk	B3PW91-TZ SMD wetoct	1.42	[1.13, 1.70]	1.34	[1.07, 1.61]	1.34	[1.07, 1.61]	0.55	[0.12, 0.89]	0.70	[0.24, 1.19]	0.56	[0.12, 0.92]	-0.00	[-0.00, -0.00]
4p2ph	DLPNO-Solv-ccCA	1.44	[0.84, 1.96]	1.12	[0.63, 1.69]	1.04	[0.47, 1.68]								

ID	name	RMSE		MAE		ME		R <sup>2</sup>		m		$\tau$		ES	
sqosi	MD-AMBER-dryoct	1.69	[1.09, 2.17]	1.42	[0.86, 1.96]	-1.40	[-1.94, -0.82]	0.51	[0.06, 0.87]	1.40	[0.41, 2.11]	0.45	[0.00, 0.84]	0.72	[0.39, 1.02]
rs4ns	BLYP/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.71	[1.14, 2.25]	1.44	[0.94, 1.99]	1.44	[0.94, 1.99]	0.06	[0.00, 0.49]	-0.19	[-0.67, 0.30]	-0.22	[-0.69, 0.36]	0.07	[-0.00, 0.25]
REF07	YANK-GAFF-tip3p-dry-oct	1.73	[0.45, 2.89]	0.95	[0.31, 2.04]	-0.75	[-1.88, -0.02]	0.22	[0.01, 0.87]	1.23	[0.28, 2.46]	0.49	[0.08, 0.88]	1.23	[0.96, 1.45]
c7t5j	PBE/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.73	[1.20, 2.28]	1.47	[1.00, 2.06]	1.47	[1.00, 2.06]	0.05	[0.00, 0.50]	-0.18	[-0.74, 0.31]	-0.16	[-0.68, 0.42]	-0.00	[-0.00, 0.05]
REF08	YANK-SMIRNOFF-TIP3P-dry-oct	1.74	[0.55, 2.85]	1.05	[0.49, 1.96]	-0.83	[-1.82, -0.13]	0.08	[0.00, 0.69]	0.65	[-0.36, 1.64]	0.31	[-0.18, 0.75]	1.22	[0.96, 1.41]
jc68f	PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.74	[1.13, 2.27]	1.47	[0.98, 2.05]	1.47	[0.98, 2.05]	0.05	[0.00, 0.49]	-0.18	[-0.73, 0.32]	-0.16	[-0.63, 0.43]	-0.00	[-0.00, 0.07]
03cyy	Linear Regression-B3LYP/6-311G**	1.75	[0.57, 2.69]	1.11	[0.43, 1.95]	0.03	[-0.91, 1.12]	0.00	[0.00, 0.57]	0.12	[-1.04, 1.60]	0.09	[-0.61, 0.72]	0.36	[0.07, 0.70]
REF05	YANK-SMIRNOFF-TIP3P-wet-oct	1.77	[0.53, 2.89]	1.07	[0.42, 2.07]	-0.97	[-1.98, -0.26]	0.08	[0.00, 0.76]	0.63	[-0.66, 1.73]	0.35	[-0.17, 0.84]	1.18	[0.86, 1.41]
hsotx	B3LYP/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.81	[1.21, 2.29]	1.56	[1.01, 2.09]	1.56	[1.01, 2.09]	0.07	[0.00, 0.47]	-0.19	[-0.61, 0.26]	-0.20	[-0.65, 0.39]	-0.00	[-0.00, 0.01]
ke5gu	MD/S-MBIS-GAFF-SPCE/MBAR/	1.82	[1.31, 2.28]	1.59	[1.08, 2.12]	-1.59	[-2.11, -1.07]	0.62	[0.17, 0.89]	1.54	[0.71, 2.22]	0.53	[-0.04, 0.88]	0.49	[0.22, 0.82]
fe8ws	B3PW91/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.83	[1.22, 2.33]	1.58	[1.06, 2.13]	1.58	[1.06, 2.13]	0.06	[0.00, 0.50]	-0.18	[-0.71, 0.34]	-0.16	[-0.64, 0.45]	-0.00	[-0.00, -0.00]
mwuua	MD-LigParGen-wetoct	1.83	[1.45, 2.13]	1.73	[1.36, 2.08]	-1.73	[-2.07, -1.35]	0.41	[0.03, 0.75]	0.67	[0.13, 1.11]	0.48	[0.08, 0.84]	0.49	[0.29, 0.72]
fyx45	LogP-prediction-Drude-FEP-HuangLab	1.85	[0.71, 2.76]	1.25	[0.53, 2.20]	0.65	[-0.30, 1.86]	0.63	[0.17, 0.92]	2.63	[1.12, 3.84]	0.67	[0.14, 1.00]	0.80	[0.44, 1.14]
5t0yn	PBE0/cc-pVTZ//B3LYP-D3/cc-pVTZ	1.85	[1.31, 2.34]	1.61	[1.10, 2.15]	1.61	[1.10, 2.15]	0.06	[0.00, 0.54]	-0.18	[-0.69, 0.25]	-0.16	[-0.62, 0.47]	-0.00	[-0.00, -0.00]
6nm1t	MD-AMBER-wetoct	1.87	[1.33, 2.44]	1.65	[1.16, 2.18]	-1.65	[-2.17, -1.16]	0.42	[0.02, 0.93]	1.10	[0.19, 1.56]	0.60	[0.10, 1.00]	0.57	[0.35, 0.82]
eufcy	MD-LigParGen-dryoct	1.99	[1.61, 2.35]	1.88	[1.49, 2.27]	-1.77	[-2.25, -1.13]	0.54	[0.18, 0.90]	1.43	[0.49, 2.49]	0.66	[0.24, 0.96]	0.41	[0.23, 0.65]
tzzb5	Alchemical-CGenFF	2.12	[1.53, 2.60]	1.87	[1.25, 2.48]	1.43	[0.52, 2.34]	0.20	[0.00, 0.59]	-0.76	[-1.61, 0.33]	-0.20	[-0.60, 0.32]	0.66	[0.35, 0.95]
3oqhx	MD-CHARMM-dryoct	2.14	[1.28, 2.85]	1.64	[0.86, 2.46]	1.11	[0.03, 2.20]	0.03	[0.00, 0.36]	-0.44	[-1.89, 0.90]	0.00	[-0.48, 0.52]	0.75	[0.37, 1.09]
bzeez	FS-AGM (Fast switching Annihilation/Growth Met...	2.20	[1.81, 2.53]	2.07	[1.57, 2.49]	-2.07	[-2.48, -1.56]	0.63	[0.17, 0.95]	1.39	[0.81, 1.98]	0.53	[-0.02, 0.91]	0.23	[0.06, 0.50]
ynquk	TWOVAR	2.26	[1.85, 2.60]	2.13	[1.66, 2.56]	2.13	[1.66, 2.56]	0.08	[0.00, 0.76]	0.25	[-0.25, 0.64]	0.38	[-0.10, 0.79]	1.07	[0.95, 1.20]
5svjv	FS-GM (Fast switching Growth Method)	2.26	[1.85, 2.66]	2.14	[1.69, 2.56]	-2.03	[-2.55, -1.37]	0.39	[0.03, 0.93]	1.20	[0.43, 1.76]	0.44	[-0.14, 0.92]	0.74	[0.56, 0.96]
odex0	InterX_ARROW_2017_PIMD_SOLVENT2_WET_OCTANOL	2.29	[1.61, 2.84]	1.98	[1.31, 2.70]	1.73	[0.87, 2.58]	0.09	[0.00, 0.63]	-0.53	[-1.70, 0.81]	-0.09	[-0.60, 0.52]	1.09	[0.91, 1.29]
pnc4j	LogP-prediction-Drude-Umbrella-HuangLab	2.29	[1.64, 2.87]	2.03	[1.38, 2.64]	2.03	[1.38, 2.64]	0.04	[0.00, 0.60]	0.31	[-0.73, 1.21]	0.20	[-0.32, 0.69]	0.39	[0.16, 0.73]
padym	InterX_ARROW_2017_PIMD_WET_OCTANOL	2.29	[1.65, 2.84]	1.99	[1.30, 2.71]	1.72	[0.77, 2.59]	0.12	[0.00, 0.65]	-0.60	[-1.87, 0.75]	-0.13	[-0.69, 0.49]	1.09	[0.90, 1.28]
REF06	YANK-SMIRNOFF-OPC-wet-oct	2.33	[1.23, 3.48]	1.85	[1.19, 2.87]	-1.85	[-2.86, -1.19]	0.13	[0.00, 0.87]	0.82	[-0.40, 1.86]	0.44	[-0.04, 0.82]	0.85	[0.59, 1.07]
REF03	YANK-GAFF-OPC-wet-oct	2.35	[1.17, 3.38]	1.85	[1.11, 2.74]	-1.85	[-2.73, -1.10]	0.13	[0.00, 0.82]	0.85	[-0.71, 2.09]	0.35	[-0.36, 0.88]	0.84	[0.54, 1.11]
REF01	YANK-GAFF-TIP3P-FB-wet-oct	2.40	[1.15, 3.78]	1.82	[1.09, 3.05]	-1.82	[-3.03, -1.07]	0.15	[0.00, 0.83]	0.99	[-0.25, 2.16]	0.42	[-0.08, 0.79]	0.88	[0.62, 1.12]
fcspk	ARROW_2017_PIMD_SOLVENT2	2.40	[1.73, 2.94]	2.10	[1.37, 2.78]	1.97	[1.11, 2.78]	0.11	[0.00, 0.63]	-0.50	[-1.59, 0.62]	-0.16	[-0.64, 0.41]	1.06	[0.86, 1.26]
REF04	YANK-SMIRNOFF-TIP3P-FB-wet-oct	2.41	[1.23, 3.59]	1.81	[0.99, 2.89]	-1.81	[-2.87, -0.97]	0.17	[0.00, 0.70]	1.09	[-0.52, 2.15]	0.27	[-0.22, 0.64]	0.85	[0.55, 1.13]
6cm6a	ARROW_2017_PIMD	2.41	[1.73, 2.94]	2.10	[1.40, 2.79]	1.94	[1.08, 2.77]	0.19	[0.00, 0.67]	-0.66	[-1.66, 0.37]	-0.27	[-0.70, 0.35]	1.06	[0.84, 1.26]
bq6fo	Extended solvent-contact model approach	2.58	[1.70, 3.35]	2.15	[1.31, 3.04]	1.55	[0.37, 2.80]	0.10	[0.00, 0.59]	1.05	[-0.84, 2.76]	0.09	[-0.35, 0.64]	0.23	[-0.00, 0.41]
4nfzz	MD/S-HI-GAFF-TIP3P/MBAR/	2.67	[1.98, 3.32]	2.44	[1.83, 3.05]	-2.44	[-3.04, -1.82]	0.40	[0.04, 0.89]	1.30	[0.54, 1.90]	0.42	[-0.14, 0.88]	0.20	[0.05, 0.37]
623c0	MD-OPLSAA-wetoct	2.67	[2.10, 3.26]	2.53	[2.05, 3.09]	-2.53	[-3.08, -2.05]	0.22	[0.00, 0.79]	0.64	[-0.08, 1.12]	0.38	[-0.17, 0.84]	0.18	[0.09, 0.29]
eg52i	ARROW_2017	2.86	[1.97, 3.56]	2.41	[1.45, 3.31]	2.06	[0.80, 3.18]	0.15	[0.00, 0.56]	-0.94	[-2.23, 0.35]	-0.16	[-0.63, 0.29]	0.96	[0.71, 1.22]
5585v	Alchemical-CGenFF	2.88	[2.02, 3.69]	2.55	[1.82, 3.40]	2.40	[1.46, 3.36]	0.04	[0.00, 0.57]	-0.41	[-2.09, 0.63]	-0.20	[-0.76, 0.35]	0.46	[0.22, 0.74]
cp8kv	MD-OPLSAA-dryoct	2.88	[2.32, 3.59]	2.72	[2.28, 3.33]	-2.72	[-3.32, -2.27]	0.24	[0.00, 0.93]	0.78	[-0.08, 1.45]	0.59	[0.12, 1.00]	0.12	[0.06, 0.22]
j4nb3	FOURVAR	2.89	[2.33, 3.34]	2.63	[1.86, 3.27]	2.63	[1.86, 3.27]	0.01	[0.00, 0.73]	0.12	[-0.74, 0.88]	0.16	[-0.35, 0.76]	0.89	[0.71, 1.09]
hf4wj	MD/S-HI-GAFF-SPCE/MBAR/	3.28	[2.47, 4.11]	3.04	[2.33, 3.82]	-3.04	[-3.80, -2.32]	0.34	[0.02, 0.85]	1.31	[0.46, 1.92]	0.38	[-0.17, 0.88]	0.09	[0.01, 0.20]
pku5g	SAMPL5_49_retro3	4.87	[4.06, 5.68]	4.68	[3.90, 5.55]	4.68	[3.90, 5.55]	0.49	[0.03, 0.90]	1.80	[0.29, 2.98]	0.56	[0.04, 1.00]	0.39	[0.25, 0.57]
po4g2	SAMPL5_49	5.46	[4.35, 6.64]	5.17	[4.19, 6.24]	5.17	[4.19, 6.24]	0.51	[0.05, 0.89]	2.33	[0.51, 3.74]	0.56	[0.04, 0.96]	0.34	[0.18, 0.51]

## 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.