ID	name	RMSE	MAE	ME	R^2	m	τ	ES
EXT09	clogP (Biobyte)	0.23 [0.16, 0.29]	0.17 [0.12, 0.23]	0.01 [-0.07, 0.10]	0.94 [0.86, 0.98]	0.94 [0.80, 1.02]	0.85 [0.75, 0.93]	0.27 [0.08, 0.42]
EXT12	MoKa_logP	0.28 [0.20, 0.35]	0.22 [0.16, 0.28]	0.03 [-0.07, 0.13]	0.91 [0.82, 0.97]	0.93 [0.76, 1.05]	0.83 [0.73, 0.91]	0.23 [0.07, 0.39]
EXT11	logP(o/w) (MOE)	0.32 [0.22, 0.41]	0.24 [0.17, 0.33]	0.11 [-0.01, 0.22]	0.90 [0.81, 0.95]	0.85 [0.74, 1.02]	0.80 [0.66, 0.91]	0.28 [0.10, 0.49]
EXT10	h_logP (MOE)	0.43 [0.34, 0.51]	0.35 [0.26, 0.45]	0.17 [0.02, 0.32]	0.83 [0.62, 0.93]	0.91 [0.67, 1.06]	0.74 [0.55, 0.90]	0.09 [0.01, 0.24]
EXT13	SlogP (MOE)	0.59 [0.48, 0.69]	0.49 [0.36, 0.61]	0.28 [0.08, 0.47]	0.71 [0.41, 0.87]	0.84 [0.60, 1.03]	0.55 [0.33, 0.73]	0.13 [0.01, 0.26]
EXT08	YANK-SMIRNOFF-tip3p-dry-oct	1.26 [0.88, 1.60]	0.97 [0.69, 1.28]	-0.85 [-1.20, -0.50]	0.56 [0.16, 0.83]	1.12 [0.59, 1.48]	0.50 [0.23, 0.73]	1.15 [0.98, 1.30]
EXT07	YANK-GAFF-tip3p-dry-oct	1.27 [0.69, 1.74]	0.88 [0.57, 1.26]	-0.74 [-1.15, -0.38]	0.55 [0.19, 0.88]	1.21 [0.80, 1.63]	0.60 [0.34, 0.81]	1.22 [1.05, 1.37]
EXT02	YANK-GAFF-TIP3P-wet-oct	1.38 [0.94, 1.78]	1.03 [0.70, 1.40]	-0.98 [-1.37, -0.63]	0.58 [0.26, 0.83]	1.21 [0.83, 1.66]	0.58 [0.35, 0.78]	1.12 [0.94, 1.28]
EXT05	YANK-SMIRNOFF-TIP3P-wet-oct	1.50 [0.96, 1.98]	1.11 [0.75, 1.52]	-1.00 [-1.46, -0.60]	0.50 [0.13, 0.81]	1.19 [0.66, 1.62]	0.54 [0.29, 0.75]	1.11 [0.92, 1.27]

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
- τ: 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.