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 [0.74, 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, 0.14]	0.91 [0.81, 0.97]	0.93 [0.75, 1.05]	0.83 [0.72, 0.91]	0.23 [0.08, 0.41]
EXT11	logP(o/w) (MOE)	0.32 [0.22, 0.41]	0.24 [0.17, 0.32]	0.11 [-0.00, 0.22]	0.90 [0.81, 0.95]	0.85 [0.75, 1.02]	0.80 [0.66, 0.91]	0.28 [0.11, 0.48]
EXT10	h_logP (MOE)	0.43 [0.33, 0.51]	0.35 [0.26, 0.44]	0.17 [0.02, 0.32]	0.83 [0.63, 0.94]	0.91 [0.67, 1.06]	0.74 [0.55, 0.90]	0.09 [0.01, 0.25]
EXT13	SlogP (MOE)	0.59 [0.48, 0.69]	0.49 [0.36, 0.62]	0.28 [0.08, 0.48]	0.71 [0.41, 0.87]	0.84 [0.60, 1.04]	0.55 [0.34, 0.73]	0.13 [0.01, 0.26]
EXT02	YANK-GAFF-TIP3P-wet-oct	0.91 [0.72, 1.10]	0.78 [0.61, 0.96]	0.41 [0.08, 0.70]	0.58 [0.33, 0.78]	1.04 [0.66, 1.54]	0.55 [0.32, 0.73]	1.25 [1.15, 1.34]
EXT08	YANK-SMIRNOFF-TIP3P-dry-oct	1.01 [0.68, 1.34]	0.78 [0.55, 1.04]	0.39 [0.04, 0.74]	0.49 [0.11, 0.78]	0.99 [0.42, 1.44]	0.46 [0.14, 0.71]	1.25 [1.12, 1.36]
EXT05	YANK-SMIRNOFF-TIP3P-wet-oct	1.05 [0.74, 1.32]	0.82 [0.59, 1.08]	0.30 [-0.08, 0.67]	0.49 [0.15, 0.74]	1.05 [0.53, 1.53]	0.47 [0.21, 0.70]	1.22 [1.09, 1.35]
EXT07	YANK-GAFF-tip3p-dry-oct	1.05 [0.85, 1.25]	0.93 [0.74, 1.12]	0.62 [0.28, 0.93]	0.58 [0.30, 0.79]	1.07 [0.71, 1.55]	0.57 [0.32, 0.76]	1.18 [1.08, 1.29]
EXT04	YANK-SMIRNOFF-TIP3P-FB-wet-oct	1.08 [0.62, 1.48]	0.71 [0.43, 1.04]	-0.31 [-0.72, 0.06]	0.46 [0.16, 0.74]	1.02 [0.59, 1.57]	0.53 [0.28, 0.75]	1.26 [1.10, 1.39]
EXT01	YANK-GAFF-TIP3P-FB-wet-oct	1.11 [0.65, 1.51]	0.72 [0.43, 1.07]	-0.20 [-0.64, 0.19]	0.54 [0.26, 0.78]	1.23 [0.86, 1.80]	0.57 [0.34, 0.77]	1.25 [1.09, 1.40]
EXT06	YANK-SMIRNOFF-OPC-wet-oct	1.16 [0.73, 1.60]	0.83 [0.55, 1.17]	-0.10 [-0.57, 0.30]	0.45 [0.13, 0.75]	1.11 [0.71, 1.56]	0.52 [0.28, 0.71]	1.22 [1.07, 1.34]
EXT03	YANK-GAFF-OPC-wet-oct	1.28 [0.73, 1.80]	0.87 [0.56, 1.26]	-0.28 [-0.78, 0.16]	0.44 [0.10, 0.73]	1.17 [0.53, 1.81]	0.47 [0.18, 0.72]	1.21 [1.06, 1.35]

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.