

QSPR is an application of machine learning

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 - “gives computers the ability to learn without being explicitly programmed” - Arthur Samuel (1959)
 - “A computer program is said to learn from experience E with respect to some task T and some performance measure P , if its performance on T , as measured by P , improves with experience E .” -Tom Mitchell (1997)

- In Quantitative Structure-Property Relationships (QSPR)
 - Experience E: chemicals
 - Task T: predicting physical property, e.g.
 - boiling point, chromatography retention times
 - activity against a biological target = QSAR
 - ADMET (absorption, distribution, metabolism, and excretion - toxicity)
 - Performance P: correlation/error in validation set/real-world applications



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Features/Descriptors