QSPR is an application of machine learning

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- In Quantitive 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

2

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Features/Descriptors