Lipophilicity is a property that is a critical factor in the prediction of the behavior of chemicals, both in the body and environment (Kwon). There is a very high correlation between the measured lipophilicity and a given chemical's ability to efficiently cross the blood brain barrier (Clark). This means that prediction of target organs, update and distribution in vivo requires certain ranges of partition coefficients leading to this being a primary means of determining a chemical's potential as a drug (Lipinski).

The partition coefficient is usually measured by having a two phase system consisting of octanol and water and measuring the concentrations in the two phases. The concentration in octanol over the concentration in water gives the partition coefficient–P, sometimes written as K_{ow}. It is most often stored and used as a log of P–logP.

$$\log P_{\mathrm{oct/wat}} = \log\left(\frac{[\mathrm{solute}]^{\text{un-ionized}}_{\text{octanol}}}{[\mathrm{solute}]^{\text{un-ionized}}_{\text{water}}}\right).$$ (wikipedia)

The usefulness of this measure for drug discovery and other applications has ensured that there is a great deal of published experimental data. Large scale screening makes it impractical to run such experiments on every new compound and is greatly aided by predicted values. There have been many models created over the years with varying degrees of success. Some of these include decision trees(Sun H), multiple linear regressions of charged atoms(Xing and Glen) and atomic contribution(Wildmand and Crippen). Wildman and Crippen's atomic contribution method is rather prevalent and is included in the widely used chemical informatics library Rdkit.

There have been a number of machine learning methods published using Quantitative Structure-Activity Relationship–QSAR (Hansch and Leo) and Quantitative Structure-Property Relationship QSPR(in silico), which are typically specialized deep neural networks.

To analyze chemical data, structures are typically reduced to fingerprints. These fingerprints are usually a binary representation of a fixed length that given the same chemical in any orientation will generate the same fingerprint and ideally such that all bits from any given substructure of a chemical will be in the fingerprint of the full structure.

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