

Are StarDrop's P450 models QSAR models?

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No. The P450 models differ from the QSAR models, being based on simulation of the chemical reaction mechanisms which lead to the formation of metabolites. Although experimental data are used to tune the parameters of the model and validate the results, the form of the underlying model is not based on an empirical fit to a training data set and this gives greater transferability across a wide range of chemistry without loss of accuracy. Accurate modeling of the chemical reactions requires quantum mechanical simulations, which are much more computationally expensive than the descriptor calculations employed by QSAR models. Consequently, the P450 metabolism models are significantly slower, taking a couple of minutes per compound. However, identifying the most likely cause of metabolic instability for a compound can help to guide chemical modifications aimed at reducing the vulnerability.