

Can you predict the metabolic rate?

Written by Matt Segall

Tuesday, 29 September 2009 21:37 - Last Updated Tuesday, 16 February 2016 13:53

In addition to the vulnerability of individual sites on a molecule, whether a compound is metabolised, and the overall rate of metabolism, will depend upon many factors in the P450 catalytic cycle, including the affinity of the molecule for the enzyme, the rates of reduction and rates of decoupling via peroxide formation. These are currently unknowns and hence metabolic rate, as opposed to lability, cannot be predicted in general. However, for individual chemical series typically only a small number of these factors dictate the rate of product formation. In this case it is possible to build local models, using the Composite Site Lability (CSL) as a descriptor.