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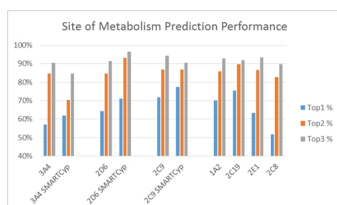
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Jon Tyzack presented this poster at the joint ISSX/JSSX North America meeting in October 2014.

Abstract:

Optibrium™, as part of the European HeCaTos project, has developed enhancements to its P450 module within StarDrop™. These include the modelling of epoxidation pathways and the capability to model the xenobiotic metabolism of an additional 4 P450 isoforms: 1A2, 2C19, 2E1 and 2C8.

The goal of the HeCaTos project is to develop integrative approaches towards highly predictive human safety assessment. The prediction of xenobiotic metabolism is an important step in this process, giving the ability to identify potential toxic metabolites. The new capability to model the formation of reactive epoxide metabolites is a vital part in this process and coupled with our new isoform specific models it enables a more complete picture of xenobiotic metabolism to be developed.



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