Dr Christopher Barber, Lhasa Limited, gave this presentation at the "Guiding Optimal Compound Design and Development Symposium" held in Cambridge, MA, USA on 19 March 2015.

Abstract

The computer-based prediction of metabolites based upon structure has a wide number of applications – from a chemist's desire to tune the metabolic profile of a lead, or a biologist's requirement to predict likely toxic metabolites, to an analyst's need to assign a peak in a bio-sample. Expert systems can provide transparent predictions with commentary and support based upon human knowledge whereas machine learning approaches are able to absorb new data more quickly but frequently show poor interpretability through the choice of descriptors and/or the model building methodology. However, these approaches are not mutually exclusive and the combination of both offers the potential for a new range of powerful predictive systems.

This talk will describe the science and results behind our work to apply machine learning approaches in order to enhance predictions made from the extensive biotransformation rule-base found within Meteor Nexus.

You can download this presentation as a PDF .