In silico predictive models are now widely used to predict a range of molecular properties and help prioritise molecule for synthesis. However, a common criticism often levelled at predictive models is that they offer few clues regarding why a molecule is predicted to have a certain property. By definition, models encode relationships between molecular structure and properties, but interpreting and visualising this information to design better molecules has been almost impossible. This is particularly true of models built with modern ‘machine learning’ techniques such as artificial neural networks (ANN), Gaussian processes (GP) or support-vector machines (SVM). The models that these techniques create have commonly been described as ‘black box.’

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In this poster we will present a novel algorithm that ‘opens’ these black box models, providing an intuitive visualisation of these structural relationships. The objectives of this approach are to:

- Clearly identify ‘problem’ regions on a molecule
- Highlight functional groups that tend to improve a molecular property
- Understand the ‘multidimensional’ structure activity relationships (SAR) of a chemical series

This poster is available as a PDF file.