

It is relatively straightforward to produce a similar visualization to Glowing Molecule for simple linear models (where the property is calculated via a weighted sum of contributions) and some other packages can generate these. However, in practice, properties are rarely linearly related to the structural characteristics of a molecule and modern modeling techniques such as artificial neural networks, Gaussian Processes and genetic programming have been used to model non-linear relationships. These methods are commonly described as 'black box' because understanding and visualising the non-linear models these generate has been impossible. The unique algorithm underlying Glowing Molecule enables this information to be extracted and visualised in an intuitive way to help interpret the structure-activity relationships captured in these models.