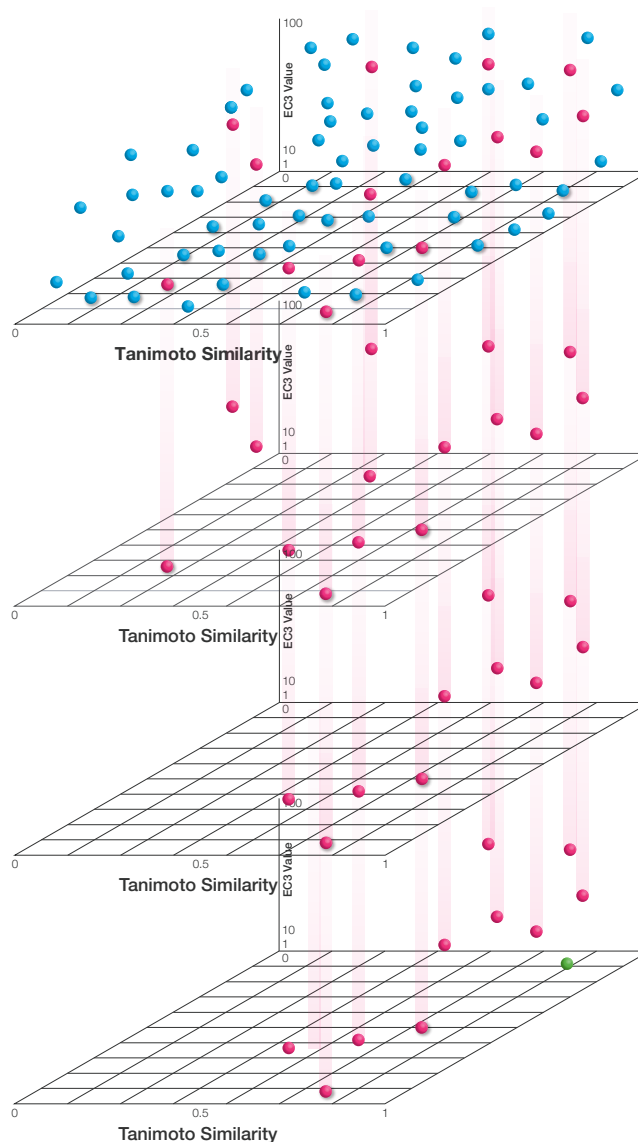


# Derek EC3 prediction methodology

Derek gives a quantitative EC3 prediction for compounds that fire a skin sensitisation alert. The prediction is derived from a Nearest Neighbour Model, where the nearest neighbours are taken from a reference set of compounds that exclusively fire the same alert as the query compound. The Tanimoto similarity score is calculated for the nearest neighbours and an EC3 prediction is made. The nearest neighbour compounds are selected from over 650 compounds in the high-quality Lhasa EC3 dataset which has been curated by Lhasa experts.

Fires Alert ●  
Doesn't Fire Alert ●  
Predicted Value ●



*The Derek Nexus  
EC3 methodology explained*

The compounds which fire the same alert as the query compound are highlighted.

The model only considers compounds that fire the alert of interest.

The model calculates the similarity of the compounds, compared to the query. The ten nearest neighbours will be used in the calculation.

These compounds are then used to make a prediction. Expert review of each prediction is recommended and the software allows the addition or removal of compounds by the user to facilitate this.