Within the chemical space of the predictive ADME QSAR model, there are a statistically significant number of data points in the independent test set, and hence the performance of the model on this set provides a good estimate of the uncertainty. For compounds outside but ‘close’ to the chemical space of the model, extrapolation beyond the training set increases the uncertainties in these predictions. Where possible, this is estimated using the performance of the model on compounds in the independent test set that lie outside of the chemical space. For compounds that differ significantly from the training set, no valid estimate of the uncertainty can be made. The uncertainty in the predictions for these compounds is reported as maximal i.e. for continuous models an infinite uncertainty and for classification models an equal probability for each class.