Each model result is provided with an estimate of the uncertainty in the prediction, in the form of a root mean square error (RMSE) for continuous data or a probability for classification data. The uncertainty is based on how similar the structure is to those molecules used when building the model. If your chemistry differs significantly from the compounds used to build the models, it is less likely that the models will be predictive and this can be seen explicitly from the uncertainties returned (see “How do you estimate uncertainties?” below). As noted above, the models supplied with StarDrop are ‘global’ and should readily distinguish ‘long range’ trends across a wide range of chemistries, but they are less likely to be able to differentiate between similar molecules in the same series.