These two models calculates the number of sp3 carbons and the total number of carbons compound. These are available to enable the calculation of properties such as saturation - the ratio of sp3 carbons to the total number of carbons (Lovering F, Bikker J, Humblet C. Escape from flatland: increasing saturation as an approach to improving clinical success. J Med Chem 2009, 52:6752–6756.). They suggest that the typical levels of saturation increase from 0.36 in drug discovery through to 0.47 in drugs.

When installed, each will appear in StarDrop in the "Models" tab alongside the ADME QSAR models and other simple properties as a "Custom" model, allowing it to be calculated easily for any data set. If you've not used custom models before, details on how to install it are available on the following pages, along with the model file...

Installation

1. Save each model file (Number of carbons.aim and Number of sp3 carbons.aim) into a directory of your choice.

2. To access the models quickly you can simply right-click on the **Models** tab in StarDrop, choose **Open Model...** and then open the saved files.

3. To ensure StarDrop always has these models available, open the **Preferences** (File->Preferences) and, in the **File Locations** tab, add the directory where the models were saved into the **Models** section.

Saturation

To calculate the saturation, run these models and use the StarDrop function editor to create a new column which calculates:

{Number of sp3 carbons}/{Number of carbons}

For a quick demonstration of how to do this take a look at this short video: