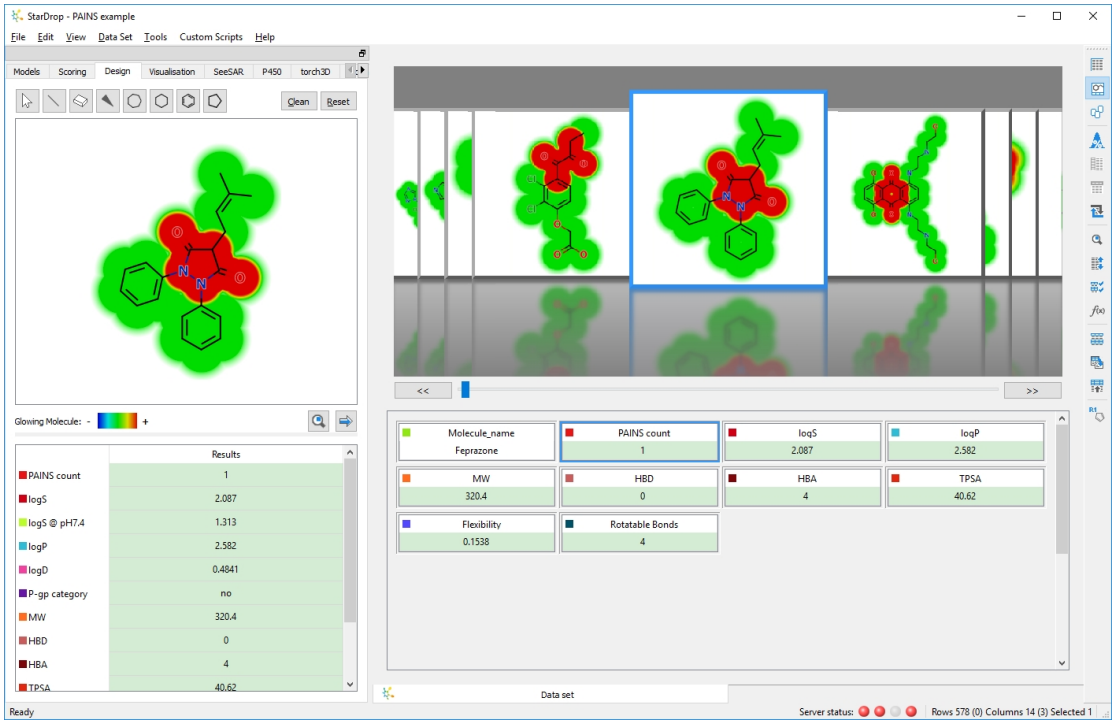
Baell and Holloway published a set of substructure filters for removal of what they termed “Pan Assay Interference Compounds (PAINS)” from screening collections [J. Med. Chem. 2010 53(7) pp. 2719-2740]. These define functional groups that are known to cause problems due to reactivity, poor development potential or known toxicity and have been widely adopted. You can download a model which calculates the number of PAINS matches for each compound here.

The original PAINS filters were defined in Sybyl Line Notation (SLN) and were converted to SMARTS by Rajarshi Guha using the Cactvs library. Rajarshi Guha notes that the conversion was not perfect.

We have created a model that can be run in StarDrop which counts the numbers of matched to PAINS substructures. Furthermore, the matches are highlighted in StarDrop's Glowing Molecule:



You can download the model for use within StarDrop from the following link:

PAINS.aim

To use the mode in StarDrop, download and save the file in a convenient place. Load itinto StarDrop using the folder button on the **Models** tab. Alternatively, the directory in which the model file has been saved can be added to the paths from which models are automatically loaded when StarDrop starts by selecting the **File->Preference** menu option and adding the directory under **Models** in the **File Locations** tab.

As an alternative, the SMARTS definitions of the PAINS substructures can be downloaded to use in StarDrop's **Filter** tool from here .