This model is based upon the following work published by Pearce et al.

Pearce BC, Sofia MJ, Good AC, Drexler DM, Stock DA. **An empirical process for the design of high-throughput screening deck filters.**
J Chem Inf Model. 2006;46:1060–1068.

Based upon the data published, this model can be downloaded and used with StarDrop 4.2 and onwards. If you've not used custom models before, details on how the model was built and how to install it are available on the following pages, along with the model file itself...

Installation

1. Save the model file (HTS promiscuity alerts.aim) into the StarDrop model files directory (in a default installation this will be "C:Program FilesStarDropmodelfiles").

2. When you start StarDrop the model will appear in the list of available models as a custom model.

Model Details

Abstract

A process for objective identification and filtering of undesirable compounds that contribute to high-throughput screening (HTS) deck promiscuity is described. Two methods of mapping hit promiscuity have been developed linking SMARTS-based structural queries with historical primary HTS data. The first compares an expected assay hit rate to actual hit rates. The second examines the propensity of an individual compound to hit multiple assays. Statistical evaluation of the data indicates a correlation between the resultant functional group filters and compound promiscuity. These data corroborate a number of commonly applied filters as well as producing some unexpected results. Application of these models to HTS collection triage reduced the number of in-house compounds considered for screening by 12%. The implications of these findings are further discussed in the context of the HTS screening set and combinatorial library design as well as compound acquisition.