

SSPROFILER

Introduction

SSPROFILER (SubStructural Profiling and Filtering) uses SMARTS-encoded substructural definitions to profile collections of structures or make selections from them. SSPROFILER is run as follows:

ssprofiler --help (to get help)

ssprofiler -i Structure.File -o Output.File -s SMARTS.File -v Vector.Binding.File -t Calculation.Type

Substructural Profiling

This mode of calculation is specified by -t profile and the output consists of structure name and the number of occurrences of each substructural target in each structure. The SMARTS file is formatted as follows (with comments specified using # as first character on the line):

SMARTS.Name SMARTS.Definition

Substructural Filtering

This mode of calculation is specified by -t filter and the output consists a file with structures that satisfy the filtering criteria. The SMARTS file is formatted as follows (with comments specified using # as first character on the line):

SMARTS.Definition Lower.Limit Upper.Limit

In order to satisfy a single SMARTS-encoded substructural requirement, the number of occurrences of matches, Number.Match, of the SMARTS target with the structure must satisfy:

Lower.Limit <= Number.Match <= Upper.Limit

Structures must satisfy every SMARTS-encoded substructural requirement in order to pass through the filter.

Vector Bindings

An optional file of vector bindings can be used both in profiling and filtering and the format of this file is as follows (with comments specified using # as first character on the line):

Vector.Binding.Name Vector.Binding.Definition