# Bayesian Model Creation Software

## 1.1 Outline

The product provided is a simple command line application that can be used to generate model files suitable for use with the StarDrop™ software. The main input is a set of SMARTS descriptors, each with an associated coefficient, which can be used to construct a PLS model for a desired property. The output is a StarDrop™ model file (*.aim) that can be loaded into the StarDrop™ client, or placed on a StarDrop™ model server.

## 1.2 Installation

No Windows installation is required. Simply copy the executable file (createmodel.exe) to the desired location. The application is built on a 32 bit platform, but should run equally well on 32 or 64 bit Windows architectures. A Linux version is not currently available.

## 1.3 Usage

```
createmodel.exe -input SomeTextFile -output NewModel [-dest C:/users/me/models
-defaulterror 2.0 -min 0.0 -max 10.0].
```

See below for explanation of parameters.

## 1.4 Parameters

### 1.4.1 Required

-input Provide the full name of a file containing the descriptor information. The file should be formatted in the same way as the file bestbins.txt supplied during the initial discussion of the project, specifically a tab-separated line for each descriptor, containing fields for BinID, SMARTS and coefficient

-output Specify the name for the model to be generated. This will appear as part of the model file name, and will be how the model is identified in the StarDrop™ UI

### 1.4.2 Optional

-dest Specify a folder where the generated model will be saved. If omitted, the destination folder will be the current working directory.

-min Specify the minimum expected value for the model output. Default is -20.0. See below for a discussion of the effect of specifying this parameter.

-max Specify the maximum expected value for the model output. Default is 20.0. See below for a discussion of the effect of specifying this parameter.

-defaulterror Specify the value to be used for the standard deviation associated with the results from the model. This value will be used by StarDrop™ when including the model results in a score calculation. The default value is 0.0.

## 1.5 Notes

### 1.5.1 Glowing Molecule™

When the generated models are used within StarDrop™ they will generate Glowing Molecule information. The intensity of the colours displayed is a function of the range of possible values for the model, as defined by the –min and –max parameters if they are specified. Reducing the range will result in more intense glows while increasing the range will reduce the intensity.

7221 Cambridge Research Park
Beach Drive, Cambridge
CB25 9TL, UK

Tel: +44 1223 815900
Fax: +44 1223 815907

Email: info@optibrium.com
Website: www.optibrium.com

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### 1.5.2 Error handling

In the following scenarios, the application will fail to generate a model:

- Command line parameters are incorrectly specified
- File containing descriptors cannot be found, or cannot be opened
- No descriptors are found when parsing the file
- A file for the generated model cannot be created at the specified location

In each of these cases, a message will be output to the screen, but no other logging is currently supported.

If individual lines of the input file cannot be parsed, the application will skip them and continue to generate a model.

The application does not attempt to validate the SMARTS patterns. If any of these are invalid, the generated model will fail to produce a result.

## 1.6 Support

chris@optibrium.com

stardrop-support@optibrium.com

## 1.7 Disclaimer

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