MBSS_DrugSim.py

MBSS_DrugSim.py is a python 3.5 script requiring the following python packages: sys, subprocess and numpy(1.11.1).
It requires MBSS_FormatTable.pl and MaBoSS

Aim
This script can be used to generate new bnd and cfg files (from a bnd and a cfg template) with new nodes representing specific targeting drugs, by inhibiting partially or completely other nodes. It then launches the simulations corresponding to the generated files. It handle single or double inhibitions.

Input
MBSS_DrugSim.py is taking as an input a config file (my_config.txt), wherein the following informations should be available in the specified order:

Model_name
List of nodes to modify separated by commas
Inhibition proportion to test separated by commas
Number of simulations to run in parallel (depending on the available cores and memory)

The Model_name should correspond to both bnd and cfg file name.
Example:
my_config_file.txt:

```
p53_MDM2_model
P53, p53h, Dam
0.0, 0.2, 0.4, 0.6, 0.8, 1.0
4
```

This example of configuration file allows the creation of bnd and cfg files containing three inhibitors (inhibiting the nodes specified line 2) and launches simulations corresponding to all the combination of double-inhibitions using all the inhibition proportions specified line 3.
It require two template files (both bnd and cfg)
Internal nodes should be specified in the template cfg file.

.istates should be specified using the following formalisms:
[Node].istate = FALSE/TRUE
[Node].istate = 0 [0], 1 [1] // 1 [0], 0 [1]
[Node].istate = 0 [1], 1 [0] // 1 [1], 0 [0]

How to run the script

In a folder, gather:

-both bnd and cfg files corresponding to the model

-your config file

MaBoSS Executable version (named as "*MaBoSS*") and MBSS_FormatTable.pl should be accessible by command line

In a terminal window located in the folder:

```
MBSS_DrugSim.py config_file_name.txt
```

Script Description

A- Create the two template bnd and cfg files (adding "new" in the names).

1- bnd modifications:

-change the logic by adding the inhibitor as an additional NAND gate

-add inhibitor nodes

2- cfg modification:

-format the istate grammar

B- Generate the bnd and cfg files corresponding to all the combination specified in the config_file with the inhibition proportions contained in my_config_file.txt (3rd line). All these combinations will be generated in a new folder: "*drug_simulations"*

C- Generate X bash scripts (task_X.sh), X corresponding to the number of parallel simulations to run. Each bash script can launch one or more simulations, depending on the total number of simulations and on the number of parallel simulations that can be launched. If needed, the bash scripts can later be launched by hand.

D- Calls the task_X.sh scripts and launches the simulations. An output and an error files will be also created, containing the console output of the simulations.
The results of the simulations will be available in /drug_simulations/name_of_the_combination, as a MBSS_FormatTable.pl output (see MBSS_FormatTable.pl documentation).