CR11: assignment 2

deadline: 4th January 2016

Please write a concise report in PDF format and send it to: russell.harmer@ens-lyon.fr

You can use gnuplot, or any other plotting software you wish, to produce the figures. If at all possible, please incorporate all figures (and Kappa rules/models) into the main body of your report.
Start by downloading GK.ka from: `http://perso.ens-lyon.fr/russell.harmer/CR11/GK.ka`

Question 1.

- Run simulations of `GK.ka` with KaSim [3000 time units should be enough; use a command line like: `kasim -i GK.ka -t 3000 -p 1000 -o output_file`] to determine the steady-state value of the observable **`S1?`** starting from initial conditions with 50, 100, 150 and 200 **`K(s)`** (with 2000 **`S(s~0)`** and 100 **`P(s)`** in each case). Plot all four simulations in the same figure.
- What do these results suggest for the overall shape of the dose-response curve of **`K()`** vs. 'the steady-state value of **`S1?`**' ?

Question 2.

Modify `GK.ka` in order to obtain, with a *single* simulation, the full dose-response curve for $0 \leq$ **`K()`** ≤ 200.

Question 3.

Further modify `GK.ka` so that **`S`** now has a second site, with a `0/1` state, whose state is modified by **`K`** and **`P`**. (Use the same rate constants as for the corresponding rules for site **`s`**.)

- What design choices did you make? What other choices could you have made?
- Define an observable **`S11?`** that tracks the number of **`S`** agents in state **`1`** for *both* sites.
- Run a *single* simulation to obtain the dose-response curve of **`K()`** vs. 'the steady-state value of **`S11?`**' for $0 \leq$ **`K()`** ≤ 200.
- Is there a difference between this curve and that of question 2? What do you think would happen if we added even more such sites to **`S`**?

Question 4.

Modify `GK.ka` (the original file, not your answers to questions 2 and 3) in order that **`K`** and **`P`** bind only those **`S`** agents that are *already* in the state that they can subsequently modify.

- Run simulations to determine the steady-state value of **`S1?`** starting from initial conditions with 50, 70, 90, 110, 130 and 150 **`K(s)`** (with 2000 **`S(s~0)`** and 100 **`P(s)`** in each case). Plot all six simulations in the same figure.
- How does the shape of these curves differ from those obtained in question 1? Can you explain why?
- What do these results suggest for the overall shape of the dose-response curve of '**`K()`**' vs. 'the steady-state value of **`S1?`**' ?

Question 5.

Further modify your answer to question 4 in order to obtain, with a *single* simulation, the full dose-response curve for $0 \leq$ **`K()`** ≤ 200. [This simulation may take quite a long time; probably 15–30 minutes.]

- Can you explain the difference between this curve and that of question 2?