

# Quick Intro to SBMLR

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April 30, 2018

## Introduction

*SBMLR* reads SBML files to and from an SBML-like R list of lists core object of class *SBML*, and it reads and writes these core objects into R text files that are well structured and light weight for editing. It also facilitates model simulations and model summaries.

## Model import, export, editing and viewing

The following code reads in Curto et al.'s purine metabolism model of 1998

```
> library(SBMLR)
> curto=readSBML(system.file("models", "curto.xml", package = "SBMLR"))
> head(summary(curto)$reactions)
```

|       | index | Laws  | initialFluxes |
|-------|-------|---|---------------|
| ada   | 1     | aada*ATP <sup>f</sup> ada4  | 2.079466999   |
| ade   | 2     | aade*Ade <sup>f</sup> ade6  | 0.009915724   |
| adna  | 3     | aadna*dATP <sup>f</sup> dnap9*dGTP <sup>f</sup> dnap10                            | 10.038261346  |
| adrnr | 4     | aadrnr*ATP <sup>f</sup> adrnr4*dATP <sup>f</sup> adrnr9*dGTP <sup>f</sup> adrnr10 | 0.201159500   |
| ampd  | 5     | aampd*ATP <sup>f</sup> fampd4*dGTP <sup>f</sup> fampd8*Pi <sup>f</sup> fampd18    | 5.640727920   |
| aprt  | 6     | aaprt*PRPP <sup>f</sup> aprt1*ATP <sup>f</sup> aprt4*Ade <sup>f</sup> aprt6       | 0.998075329   |

and the next two lines serialize the object *curto* of S3 class *SBML* (R list of lists) into a current working directory SBML (XML) file and editable R code SBMLR file. Relative to the option of using *dput* and *deparse*, *saveSBMLR* and *readSBMLR* ASCII text representations are more pleasant to look at and thus edit (the carriage returns are in the right places).

```
> saveSBML(curto,"curto.xml")
> saveSBMLR(curto,"curto.r")
```

These two files can then be read back in and compared as follows.

```
> curtoX=readSBML("curto.xml")
> curtoR=readSBMLR("curto.r")
> head((curtoX==curtoR)$species)
```

|      | index | initialConcentrations | boundaryConditions |
|------|-------|-----------------------|--------------------|
| PRPP | TRUE  | TRUE                  | TRUE               |
| IMP  | TRUE  | TRUE                  | TRUE               |
| SAMP | TRUE  | TRUE                  | TRUE               |
| ATP  | TRUE  | TRUE                  | TRUE               |
| SAM  | TRUE  | TRUE                  | TRUE               |
| Ade  | TRUE  | TRUE                  | TRUE               |

```
> head((curtoX==curtoR)$reactions)
```

|       | index | Laws | initialFluxes |
|-------|-------|------|---------------|
| ada   | TRUE  | TRUE | TRUE          |
| ade   | TRUE  | TRUE | TRUE          |
| adna  | TRUE  | TRUE | TRUE          |
| adrnr | TRUE  | TRUE | TRUE          |
| ampd  | TRUE  | TRUE | TRUE          |
| aprt  | TRUE  | TRUE | TRUE          |

Values in these two dataframes are TRUE where the initial concentrations, fluxes, and reaction rate laws (as strings) are equal.

## Model simulation

The following simulation first shows that the initial condition is a steady state. It then shows the time course response to an increase in [PRPP] from 5 uM to 50 uM.

```
> out1=sim(curto,seq(-20,0,1))
> curto$species$PRPP$ic=50
> out2=sim(curto,0:70)
> outs=data.frame(rbind(out1,out2))
> attach(outs)
> par(mfrow=c(2,1))
> plot(time,IMP,type="l",xlab="minutes",ylab="IMP (uM)")
> plot(time,HX,type="l",xlab="minutes",ylab="HX (uM)")
> par(mfrow=c(1,1))
> detach(outs)
```

The modulator argument to *sim* is either NULL, a vector of numbers, or a list of interpolation functions (time varying enzyme concentration boundary conditions). The vector and list lengths are equal to the number of reactions; in the vector case reaction rate law amplitude parameters are multiplied by 1 at times less than zero and the corresponding vector element thereafter. The following code doubles the amplitude parameters of Curto et al's 37 reactions at t=0; concentrations then stay the same as fluxes double.

```
> curto$species$PRPP$ic=5 # return PRPP IC to its original value
> sim(curto,(-10):10,modulator=rep(2,37)) # bumpless transfer in concentrations since all V
```

|    | time     | PRPP     | IMP         | SAMP      | ATP       | SAM      | Ade       | XMP      |
|----|----------|----------|-------------|-----------|-----------|----------|-----------|----------|
| 1  | -10      | 5.000000 | 98.26340    | 0.1981890 | 2475.350  | 3.991870 | 0.9847300 | 24.79300 |
| 2  | -9       | 5.017097 | 98.25819    | 0.1981848 | 2475.352  | 3.991870 | 0.9849151 | 24.79299 |
| 3  | -8       | 5.017231 | 98.25855    | 0.1981853 | 2475.354  | 3.991870 | 0.9848325 | 24.79298 |
| 4  | -7       | 5.017280 | 98.25890    | 0.1981857 | 2475.354  | 3.991871 | 0.9847894 | 24.79296 |
| 5  | -6       | 5.017315 | 98.25922    | 0.1981860 | 2475.355  | 3.991871 | 0.9847674 | 24.79295 |
| 6  | -5       | 5.017341 | 98.25951    | 0.1981863 | 2475.355  | 3.991871 | 0.9847554 | 24.79294 |
| 7  | -4       | 5.017360 | 98.25977    | 0.1981865 | 2475.354  | 3.991871 | 0.9847480 | 24.79293 |
| 8  | -3       | 5.017375 | 98.26000    | 0.1981867 | 2475.354  | 3.991871 | 0.9847433 | 24.79293 |
| 9  | -2       | 5.017386 | 98.26020    | 0.1981869 | 2475.354  | 3.991871 | 0.9847401 | 24.79292 |
| 10 | -1       | 5.017395 | 98.26039    | 0.1981870 | 2475.354  | 3.991870 | 0.9847379 | 24.79291 |
| 11 | 0        | 5.017402 | 98.26058    | 0.1981872 | 2475.354  | 3.991870 | 0.9847361 | 24.79290 |
| 12 | 1        | 5.017411 | 98.26086    | 0.1981874 | 2475.354  | 3.991870 | 0.9847342 | 24.79289 |
| 13 | 2        | 5.017415 | 98.26110    | 0.1981876 | 2475.354  | 3.991870 | 0.9847331 | 24.79288 |
| 14 | 3        | 5.017419 | 98.26131    | 0.1981877 | 2475.354  | 3.991870 | 0.9847324 | 24.79287 |
| 15 | 4        | 5.017421 | 98.26150    | 0.1981879 | 2475.354  | 3.991870 | 0.9847319 | 24.79286 |
| 16 | 5        | 5.017422 | 98.26167    | 0.1981880 | 2475.354  | 3.991870 | 0.9847317 | 24.79286 |
| 17 | 6        | 5.017422 | 98.26181    | 0.1981881 | 2475.353  | 3.991870 | 0.9847316 | 24.79285 |
| 18 | 7        | 5.017422 | 98.26194    | 0.1981882 | 2475.353  | 3.991870 | 0.9847315 | 24.79285 |
| 19 | 8        | 5.017422 | 98.26206    | 0.1981883 | 2475.353  | 3.991870 | 0.9847315 | 24.79284 |
| 20 | 9        | 5.017422 | 98.26216    | 0.1981884 | 2475.353  | 3.991870 | 0.9847315 | 24.79284 |
| 21 | 10       | 5.017422 | 98.26226    | 0.1981885 | 2475.353  | 3.991870 | 0.9847315 | 24.79284 |
|    | GTP      | dATP     | dGTP        | RNA       | DNA       | HX       | Xa        | Gua      |
| 1  | 410.2230 | 6.014130 | 3.025810    | 28680.50  | 5179.340  | 9.517850 | 5.059410  | 5.506380 |
| 2  | 410.2223 | 6.014135 | 3.025813    | 28680.50  | 5179.340  | 9.519836 | 5.059734  | 5.508591 |
| 3  | 410.2237 | 6.014136 | 3.025813    | 28680.49  | 5179.340  | 9.519291 | 5.059957  | 5.508056 |
| 4  | 410.2244 | 6.014137 | 3.025814    | 28680.49  | 5179.341  | 9.518845 | 5.060051  | 5.507660 |
| 5  | 410.2248 | 6.014137 | 3.025814    | 28680.49  | 5179.341  | 9.518494 | 5.060063  | 5.507373 |
| 6  | 410.2250 | 6.014138 | 3.025814    | 28680.49  | 5179.341  | 9.518221 | 5.060026  | 5.507162 |
| 7  | 410.2251 | 6.014138 | 3.025814    | 28680.49  | 5179.341  | 9.518010 | 5.059964  | 5.507004 |
| 8  | 410.2251 | 6.014139 | 3.025814    | 28680.49  | 5179.341  | 9.517849 | 5.059891  | 5.506887 |
| 9  | 410.2251 | 6.014139 | 3.025814    | 28680.49  | 5179.342  | 9.517728 | 5.059816  | 5.506798 |
| 10 | 410.2251 | 6.014139 | 3.025814    | 28680.49  | 5179.342  | 9.517638 | 5.059744  | 5.506731 |
| 11 | 410.2251 | 6.014140 | 3.025814    | 28680.49  | 5179.342  | 9.517565 | 5.059668  | 5.506674 |
| 12 | 410.2251 | 6.014141 | 3.025814    | 28680.49  | 5179.342  | 9.517495 | 5.059567  | 5.506611 |
| 13 | 410.2251 | 6.014142 | 3.025814    | 28680.49  | 5179.343  | 9.517470 | 5.059494  | 5.506575 |
| 14 | 410.2251 | 6.014142 | 3.025815    | 28680.49  | 5179.343  | 9.517462 | 5.059439  | 5.506549 |
| 15 | 410.2251 | 6.014143 | 3.025815    | 28680.49  | 5179.344  | 9.517471 | 5.059403  | 5.506534 |
| 16 | 410.2251 | 6.014144 | 3.025815    | 28680.49  | 5179.344  | 9.517490 | 5.059382  | 5.506526 |
| 17 | 410.2251 | 6.014145 | 3.025815    | 28680.49  | 5179.344  | 9.517515 | 5.059373  | 5.506522 |
| 18 | 410.2251 | 6.014146 | 3.025815    | 28680.49  | 5179.345  | 9.517541 | 5.059370  | 5.506520 |
| 19 | 410.2251 | 6.014147 | 3.025815    | 28680.49  | 5179.345  | 9.517566 | 5.059371  | 5.506519 |
| 20 | 410.2251 | 6.014148 | 3.025815    | 28680.49  | 5179.346  | 9.517590 | 5.059375  | 5.506519 |
| 21 | 410.2251 | 6.014148 | 3.025816    | 28680.49  | 5179.346  | 9.517612 | 5.059380  | 5.506518 |
|    | UA       | ada      | ade         | adna      | adrnr     | ampd     | aprt      |          |
| 1  | 100.2930 | 2.079467 | 0.009915724 | 10.03826  | 0.2011595 | 5.640728 | 0.9963412 |          |

|    |          |           |             |           |           |           |           |           |
|----|----------|-----------|-------------|-----------|-----------|-----------|-----------|-----------|
| 2  | 100.2931 | 2.079469  | 0.009916749 | 10.03827  | 0.2011596 | 5.640732  | 0.9981831 |           |
| 3  | 100.2932 | 2.079470  | 0.009916292 | 10.03827  | 0.2011597 | 5.640735  | 0.9981332 |           |
| 4  | 100.2933 | 2.079471  | 0.009916053 | 10.03827  | 0.2011597 | 5.640735  | 0.9981052 |           |
| 5  | 100.2935 | 2.079471  | 0.009915932 | 10.03827  | 0.2011597 | 5.640736  | 0.9980919 |           |
| 6  | 100.2936 | 2.079471  | 0.009915865 | 10.03827  | 0.2011597 | 5.640735  | 0.9980853 |           |
| 7  | 100.2938 | 2.079471  | 0.009915824 | 10.03827  | 0.2011597 | 5.640735  | 0.9980816 |           |
| 8  | 100.2939 | 2.079471  | 0.009915798 | 10.03827  | 0.2011597 | 5.640735  | 0.9980795 |           |
| 9  | 100.2940 | 2.079470  | 0.009915780 | 10.03827  | 0.2011597 | 5.640735  | 0.9980783 |           |
| 10 | 100.2940 | 2.079470  | 0.009915768 | 10.03827  | 0.2011597 | 5.640735  | 0.9980775 |           |
| 11 | 100.2941 | 4.158941  | 0.019831516 | 20.07655  | 0.4023194 | 11.281469 | 1.9961538 |           |
| 12 | 100.2941 | 4.158940  | 0.019831495 | 20.07655  | 0.4023193 | 11.281468 | 1.9961526 |           |
| 13 | 100.2940 | 4.158940  | 0.019831483 | 20.07655  | 0.4023193 | 11.281468 | 1.9961521 |           |
| 14 | 100.2940 | 4.158940  | 0.019831475 | 20.07655  | 0.4023193 | 11.281467 | 1.9961516 |           |
| 15 | 100.2939 | 4.158940  | 0.019831470 | 20.07655  | 0.4023193 | 11.281467 | 1.9961514 |           |
| 16 | 100.2939 | 4.158940  | 0.019831467 | 20.07655  | 0.4023193 | 11.281467 | 1.9961513 |           |
| 17 | 100.2938 | 4.158940  | 0.019831466 | 20.07655  | 0.4023193 | 11.281467 | 1.9961512 |           |
| 18 | 100.2937 | 4.158940  | 0.019831465 | 20.07656  | 0.4023193 | 11.281467 | 1.9961511 |           |
| 19 | 100.2937 | 4.158940  | 0.019831465 | 20.07656  | 0.4023193 | 11.281467 | 1.9961511 |           |
| 20 | 100.2936 | 4.158940  | 0.019831465 | 20.07656  | 0.4023193 | 11.281467 | 1.9961511 |           |
| 21 | 100.2936 | 4.158940  | 0.019831465 | 20.07656  | 0.4023193 | 11.281467 | 1.9961511 |           |
|    | arna     | asuc      | asli        | dada      | den       | dgnuc     | dnaa      | dnag      |
| 1  | 1985.621 | 8.003186  | 8.003185    | 0.2004510 | 2.386351  | 0.1008502 | 10.03756  | 6.826370  |
| 2  | 1985.621 | 8.003012  | 8.003012    | 0.2004511 | 2.402707  | 0.1008503 | 10.03756  | 6.826370  |
| 3  | 1985.621 | 8.003028  | 8.003027    | 0.2004512 | 2.402833  | 0.1008504 | 10.03756  | 6.826371  |
| 4  | 1985.622 | 8.003042  | 8.003041    | 0.2004512 | 2.402879  | 0.1008504 | 10.03756  | 6.826371  |
| 5  | 1985.622 | 8.003053  | 8.003053    | 0.2004512 | 2.402911  | 0.1008504 | 10.03756  | 6.826371  |
| 6  | 1985.622 | 8.003064  | 8.003063    | 0.2004512 | 2.402935  | 0.1008504 | 10.03756  | 6.826371  |
| 7  | 1985.622 | 8.003072  | 8.003072    | 0.2004512 | 2.402953  | 0.1008504 | 10.03756  | 6.826372  |
| 8  | 1985.622 | 8.003080  | 8.003080    | 0.2004512 | 2.402967  | 0.1008504 | 10.03756  | 6.826372  |
| 9  | 1985.622 | 8.003087  | 8.003087    | 0.2004513 | 2.402977  | 0.1008504 | 10.03756  | 6.826372  |
| 10 | 1985.622 | 8.003093  | 8.003093    | 0.2004513 | 2.402985  | 0.1008504 | 10.03756  | 6.826372  |
| 11 | 3971.245 | 16.006199 | 16.006199   | 0.4009026 | 4.805985  | 0.2017008 | 20.07513  | 13.652746 |
| 12 | 3971.245 | 16.006217 | 16.006217   | 0.4009026 | 4.806000  | 0.2017008 | 20.07513  | 13.652747 |
| 13 | 3971.245 | 16.006233 | 16.006233   | 0.4009027 | 4.806008  | 0.2017008 | 20.07513  | 13.652748 |
| 14 | 3971.245 | 16.006247 | 16.006247   | 0.4009027 | 4.806014  | 0.2017008 | 20.07513  | 13.652749 |
| 15 | 3971.245 | 16.006260 | 16.006259   | 0.4009028 | 4.806017  | 0.2017008 | 20.07514  | 13.652750 |
| 16 | 3971.245 | 16.006270 | 16.006270   | 0.4009028 | 4.806018  | 0.2017008 | 20.07514  | 13.652751 |
| 17 | 3971.245 | 16.006280 | 16.006280   | 0.4009029 | 4.806019  | 0.2017008 | 20.07514  | 13.652752 |
| 18 | 3971.245 | 16.006288 | 16.006288   | 0.4009030 | 4.806018  | 0.2017008 | 20.07514  | 13.652753 |
| 19 | 3971.245 | 16.006296 | 16.006296   | 0.4009030 | 4.806018  | 0.2017008 | 20.07514  | 13.652754 |
| 20 | 3971.245 | 16.006303 | 16.006303   | 0.4009031 | 4.806018  | 0.2017009 | 20.07514  | 13.652755 |
| 21 | 3971.245 | 16.006309 | 16.006309   | 0.4009031 | 4.806017  | 0.2017009 | 20.07515  | 13.652756 |
|    | gdna     | gdrnr     | gmpr        | gmpr      | gnuc      | gprt      | grna      | gua       |
| 1  | 6.825859 | 0.1003440 | 0.5138721   | 1.595763  | 4.807078  | 3.738009  | 1323.532  | 1.154277  |
| 2  | 6.825863 | 0.1003438 | 0.5138758   | 1.595763  | 4.807071  | 3.753992  | 1323.532  | 1.154508  |
| 3  | 6.825864 | 0.1003439 | 0.5138768   | 1.595763  | 4.807085  | 3.753944  | 1323.532  | 1.154452  |

|    |           |            |           |          |          |            |          |          |
|----|-----------|------------|-----------|----------|----------|------------|----------|----------|
| 4  | 6.825864  | 0.1003440  | 0.5138774 | 1.595763 | 4.807093 | 3.753867   | 1323.533 | 1.154411 |
| 5  | 6.825865  | 0.1003440  | 0.5138776 | 1.595763 | 4.807097 | 3.753812   | 1323.533 | 1.154381 |
| 6  | 6.825865  | 0.1003440  | 0.5138777 | 1.595763 | 4.807099 | 3.753773   | 1323.533 | 1.154359 |
| 7  | 6.825865  | 0.1003440  | 0.5138778 | 1.595762 | 4.807100 | 3.753744   | 1323.533 | 1.154342 |
| 8  | 6.825866  | 0.1003440  | 0.5138777 | 1.595762 | 4.807100 | 3.753723   | 1323.533 | 1.154330 |
| 9  | 6.825866  | 0.1003440  | 0.5138777 | 1.595762 | 4.807101 | 3.753708   | 1323.533 | 1.154320 |
| 10 | 6.825866  | 0.1003440  | 0.5138777 | 1.595762 | 4.807101 | 3.753696   | 1323.533 | 1.154313 |
| 11 | 13.651733 | 0.2006880  | 1.0277554 | 3.191524 | 9.614202 | 7.507373   | 2647.066 | 2.308615 |
| 12 | 13.651734 | 0.2006880  | 1.0277553 | 3.191524 | 9.614202 | 7.507352   | 2647.066 | 2.308602 |
| 13 | 13.651735 | 0.2006879  | 1.0277552 | 3.191524 | 9.614202 | 7.507340   | 2647.066 | 2.308594 |
| 14 | 13.651736 | 0.2006879  | 1.0277552 | 3.191524 | 9.614201 | 7.507331   | 2647.066 | 2.308589 |
| 15 | 13.651737 | 0.2006878  | 1.0277551 | 3.191523 | 9.614201 | 7.507326   | 2647.066 | 2.308586 |
| 16 | 13.651738 | 0.2006878  | 1.0277551 | 3.191523 | 9.614201 | 7.507323   | 2647.066 | 2.308584 |
| 17 | 13.651739 | 0.2006878  | 1.0277550 | 3.191523 | 9.614201 | 7.507322   | 2647.066 | 2.308583 |
| 18 | 13.651740 | 0.2006877  | 1.0277549 | 3.191523 | 9.614201 | 7.507321   | 2647.066 | 2.308583 |
| 19 | 13.651741 | 0.2006877  | 1.0277549 | 3.191523 | 9.614201 | 7.507320   | 2647.066 | 2.308582 |
| 20 | 13.651742 | 0.2006876  | 1.0277548 | 3.191523 | 9.614201 | 7.507320   | 2647.066 | 2.308582 |
| 21 | 13.651743 | 0.2006876  | 1.0277547 | 3.191523 | 9.614201 | 7.507320   | 2647.066 | 2.308582 |
|    | hprt      | hx         | hxd       | impd     | inuc     | mat        | polyam   | prpps    |
| 1  | 3.669760  | 0.04730928 | 1.191281  | 1.595762 | 2.642505 | 14.98849   | 1.007991 | 20.88492 |
| 2  | 3.684109  | 0.04732034 | 1.191443  | 1.595750 | 2.642393 | 14.98850   | 1.007991 | 20.88278 |
| 3  | 3.684104  | 0.04731730 | 1.191398  | 1.595751 | 2.642401 | 14.98850   | 1.007991 | 20.88275 |
| 4  | 3.684049  | 0.04731482 | 1.191362  | 1.595751 | 2.642409 | 14.98850   | 1.007991 | 20.88274 |
| 5  | 3.684001  | 0.04731287 | 1.191333  | 1.595752 | 2.642416 | 14.98850   | 1.007991 | 20.88274 |
| 6  | 3.683961  | 0.04731135 | 1.191311  | 1.595753 | 2.642422 | 14.98850   | 1.007991 | 20.88273 |
| 7  | 3.683929  | 0.04731017 | 1.191294  | 1.595754 | 2.642427 | 14.98850   | 1.007991 | 20.88273 |
| 8  | 3.683904  | 0.04730928 | 1.191281  | 1.595754 | 2.642432 | 14.98850   | 1.007991 | 20.88273 |
| 9  | 3.683883  | 0.04730860 | 1.191271  | 1.595755 | 2.642437 | 14.98850   | 1.007991 | 20.88273 |
| 10 | 3.683868  | 0.04730810 | 1.191264  | 1.595755 | 2.642441 | 14.98850   | 1.007991 | 20.88273 |
| 11 | 7.367707  | 0.09461539 | 2.382516  | 3.191511 | 5.284890 | 29.97699   | 2.015983 | 41.76545 |
| 12 | 7.367676  | 0.09461462 | 2.382504  | 3.191513 | 5.284902 | 29.97699   | 2.015983 | 41.76545 |
| 13 | 7.367658  | 0.09461434 | 2.382500  | 3.191514 | 5.284912 | 29.97699   | 2.015983 | 41.76545 |
| 14 | 7.367646  | 0.09461425 | 2.382499  | 3.191515 | 5.284921 | 29.97699   | 2.015983 | 41.76545 |
| 15 | 7.367640  | 0.09461435 | 2.382500  | 3.191516 | 5.284929 | 29.97699   | 2.015983 | 41.76545 |
| 16 | 7.367638  | 0.09461456 | 2.382503  | 3.191517 | 5.284936 | 29.97699   | 2.015983 | 41.76545 |
| 17 | 7.367638  | 0.09461483 | 2.382507  | 3.191518 | 5.284943 | 29.97699   | 2.015983 | 41.76545 |
| 18 | 7.367639  | 0.09461512 | 2.382512  | 3.191519 | 5.284948 | 29.97699   | 2.015983 | 41.76545 |
| 19 | 7.367641  | 0.09461540 | 2.382516  | 3.191519 | 5.284953 | 29.97699   | 2.015983 | 41.76545 |
| 20 | 7.367642  | 0.09461567 | 2.382520  | 3.191520 | 5.284958 | 29.97699   | 2.015983 | 41.76545 |
| 21 | 7.367644  | 0.09461592 | 2.382523  | 3.191520 | 5.284962 | 29.97699   | 2.015983 | 41.76545 |
|    | pyr       | rnaa       | rnag      | trans    | ua       | x          | xd       | R5P Pi   |
| 1  | 9.99989   | 1985.551   | 1323.605  | 13.98050 | 2.314825 | 0.03071716 | 2.314841 | 18 1400  |
| 2  | 10.04334  | 1985.551   | 1323.605  | 13.98050 | 2.314828 | 0.03072109 | 2.314923 | 18 1400  |
| 3  | 10.04368  | 1985.551   | 1323.605  | 13.98050 | 2.314834 | 0.03072380 | 2.314979 | 18 1400  |
| 4  | 10.04380  | 1985.550   | 1323.605  | 13.98050 | 2.314842 | 0.03072494 | 2.315002 | 18 1400  |
| 5  | 10.04389  | 1985.550   | 1323.605  | 13.98050 | 2.314850 | 0.03072508 | 2.315005 | 18 1400  |

```

6 10.04396 1985.550 1323.605 13.98050 2.314858 0.03072464 2.314996 18 1400
7 10.04401 1985.550 1323.605 13.98050 2.314864 0.03072389 2.314980 18 1400
8 10.04404 1985.550 1323.605 13.98050 2.314870 0.03072300 2.314962 18 1400
9 10.04407 1985.550 1323.605 13.98050 2.314874 0.03072209 2.314943 18 1400
10 10.04409 1985.550 1323.605 13.98050 2.314877 0.03072121 2.314925 18 1400
11 20.08822 3971.101 2647.209 27.96101 4.629758 0.06144059 4.629812 18 1400
12 20.08827 3971.101 2647.209 27.96101 4.629760 0.06143812 4.629761 18 1400
13 20.08829 3971.101 2647.209 27.96101 4.629757 0.06143636 4.629724 18 1400
14 20.08831 3971.101 2647.209 27.96101 4.629753 0.06143501 4.629696 18 1400
15 20.08832 3971.101 2647.209 27.96101 4.629747 0.06143415 4.629678 18 1400
16 20.08832 3971.101 2647.209 27.96101 4.629740 0.06143363 4.629668 18 1400
17 20.08832 3971.101 2647.209 27.96101 4.629732 0.06143340 4.629663 18 1400
18 20.08832 3971.101 2647.209 27.96101 4.629725 0.06143334 4.629662 18 1400
19 20.08832 3971.101 2647.209 27.96101 4.629719 0.06143337 4.629662 18 1400
20 20.08832 3971.101 2647.209 27.96101 4.629714 0.06143346 4.629664 18 1400
21 20.08832 3971.101 2647.209 27.96101 4.629709 0.06143358 4.629667 18 1400

```

If half the fluxes increase and the other half decrease, both by 10 percent, both concentrations and fluxes change

```
> sim(curto,(-10):10,modulator=c(rep(1.1,20),rep(0.9,17))) # half up, half down, not bumps
```

|    | time | PRPP      | IMP       | SAMP        | ATP        | SAM      | Ade          |
|----|------|-----------|-----------|-------------|------------|----------|--------------|
| 1  | -10  | 5.000000  | 98.26340  | 0.198189000 | 2475.35000 | 3.991870 | 0.9847300000 |
| 2  | -9   | 5.017097  | 98.25819  | 0.198184839 | 2475.35234 | 3.991870 | 0.9849150719 |
| 3  | -8   | 5.017231  | 98.25855  | 0.198185337 | 2475.35377 | 3.991870 | 0.9848325423 |
| 4  | -7   | 5.017280  | 98.25890  | 0.198185738 | 2475.35440 | 3.991871 | 0.9847893888 |
| 5  | -6   | 5.017315  | 98.25922  | 0.198186049 | 2475.35459 | 3.991871 | 0.9847674154 |
| 6  | -5   | 5.017341  | 98.25951  | 0.198186302 | 2475.35458 | 3.991871 | 0.9847553831 |
| 7  | -4   | 5.017360  | 98.25977  | 0.198186517 | 2475.35449 | 3.991871 | 0.9847479991 |
| 8  | -3   | 5.017375  | 98.26000  | 0.198186702 | 2475.35438 | 3.991871 | 0.9847432878 |
| 9  | -2   | 5.017386  | 98.26020  | 0.198186865 | 2475.35426 | 3.991871 | 0.9847401086 |
| 10 | -1   | 5.017395  | 98.26039  | 0.198187011 | 2475.35415 | 3.991870 | 0.9847378781 |
| 11 | 0    | 5.017401  | 98.26056  | 0.198187143 | 2475.35388 | 3.991870 | 0.9847361680 |
| 12 | 1    | 4.942532  | 97.64982  | 0.176888021 | 2097.34855 | 3.897049 | 0.8013941149 |
| 13 | 2    | 5.263281  | 96.43286  | 0.156424689 | 1747.81132 | 3.757779 | 0.6111148919 |
| 14 | 3    | 5.678426  | 94.79494  | 0.136079555 | 1418.61369 | 3.604306 | 0.4334451343 |
| 15 | 4    | 6.207959  | 92.84139  | 0.115207395 | 1106.99434 | 3.431282 | 0.2850700703 |
| 16 | 5    | 6.906082  | 90.75058  | 0.093546041 | 813.84695  | 3.229754 | 0.1708405090 |
| 17 | 6    | 7.882141  | 88.89321  | 0.071072057 | 543.51880  | 2.985496 | 0.0889365122 |
| 18 | 7    | 9.370363  | 88.20399  | 0.048063715 | 305.51368  | 2.672649 | 0.0360755833 |
| 19 | 8    | 11.954152 | 91.78347  | 0.025759482 | 120.34109  | 2.240165 | 0.0088246789 |
| 20 | 9    | 16.535108 | 113.03875 | 0.010344786 | 28.62137   | 1.668577 | 0.0010455917 |
| 21 | 10   | 19.417926 | 167.86461 | 0.007564066 | 14.10887   | 1.380950 | 0.0003501161 |

  

|   | XMP      | GTP      | dATP     | dGTP     | RNA      | DNA      | HX        | Xa       |
|---|----------|----------|----------|----------|----------|----------|-----------|----------|
| 1 | 24.79300 | 410.2230 | 6.014130 | 3.025810 | 28680.50 | 5179.340 | 9.5178500 | 5.059410 |
| 2 | 24.79299 | 410.2223 | 6.014135 | 3.025813 | 28680.50 | 5179.340 | 9.5198361 | 5.059734 |

|    |           |           |            |              |           |           |            |          |
|----|-----------|-----------|------------|--------------|-----------|-----------|------------|----------|
| 3  | 24.79298  | 410.2237  | 6.014136   | 3.025813     | 28680.49  | 5179.340  | 9.5192907  | 5.059957 |
| 4  | 24.79296  | 410.2244  | 6.014137   | 3.025814     | 28680.49  | 5179.341  | 9.5188453  | 5.060051 |
| 5  | 24.79295  | 410.2248  | 6.014137   | 3.025814     | 28680.49  | 5179.341  | 9.5184941  | 5.060063 |
| 6  | 24.79294  | 410.2250  | 6.014138   | 3.025814     | 28680.49  | 5179.341  | 9.5182207  | 5.060026 |
| 7  | 24.79293  | 410.2251  | 6.014138   | 3.025814     | 28680.49  | 5179.341  | 9.5180098  | 5.059964 |
| 8  | 24.79293  | 410.2251  | 6.014139   | 3.025814     | 28680.49  | 5179.341  | 9.5178489  | 5.059891 |
| 9  | 24.79292  | 410.2251  | 6.014139   | 3.025814     | 28680.49  | 5179.342  | 9.5177278  | 5.059816 |
| 10 | 24.79291  | 410.2251  | 6.014139   | 3.025814     | 28680.49  | 5179.342  | 9.5176378  | 5.059744 |
| 11 | 24.79290  | 410.2251  | 6.014140   | 3.025814     | 28680.49  | 5179.342  | 9.5175724  | 5.059678 |
| 12 | 24.49250  | 421.2806  | 6.012598   | 3.026378     | 29048.29  | 5179.342  | 9.8442789  | 5.089136 |
| 13 | 24.22829  | 449.4006  | 6.007925   | 3.029316     | 29371.93  | 5179.341  | 9.6202453  | 5.150115 |
| 14 | 24.00079  | 489.6995  | 5.999332   | 3.035442     | 29664.27  | 5179.341  | 8.8685370  | 5.210558 |
| 15 | 23.81308  | 540.3000  | 5.985949   | 3.045132     | 29929.96  | 5179.342  | 7.6661551  | 5.253871 |
| 16 | 23.67127  | 601.3383  | 5.966942   | 3.058752     | 30168.06  | 5179.346  | 6.1110016  | 5.268422 |
| 17 | 23.58600  | 674.7570  | 5.941320   | 3.076824     | 30372.58  | 5179.352  | 4.3426651  | 5.243664 |
| 18 | 23.57648  | 765.0964  | 5.907563   | 3.100206     | 30530.09  | 5179.361  | 2.5826310  | 5.171136 |
| 19 | 23.68077  | 882.3175  | 5.862875   | 3.130442     | 30611.69  | 5179.371  | 1.1867220  | 5.052040 |
| 20 | 23.97258  | 1045.5194 | 5.802620   | 3.170440     | 30562.35  | 5179.380  | 0.5824035  | 4.920737 |
| 21 | 24.46735  | 1241.2306 | 5.730538   | 3.222250     | 30416.42  | 5179.387  | 0.9059277  | 4.892631 |
|    | Gua       | UA        | ada        | ade          | adna      | adrnr     | ampd       |          |
| 1  | 5.506380  | 100.2930  | 2.07946700 | 0.0099157243 | 10.03826  | 0.2011595 | 5.64072792 |          |
| 2  | 5.508591  | 100.2931  | 2.07946890 | 0.0099167492 | 10.03827  | 0.2011596 | 5.64073245 |          |
| 3  | 5.508056  | 100.2932  | 2.07947007 | 0.0099162922 | 10.03827  | 0.2011597 | 5.64073451 |          |
| 4  | 5.507660  | 100.2933  | 2.07947058 | 0.0099160532 | 10.03827  | 0.2011597 | 5.64073535 |          |
| 5  | 5.507373  | 100.2935  | 2.07947074 | 0.0099159315 | 10.03827  | 0.2011597 | 5.64073555 |          |
| 6  | 5.507162  | 100.2936  | 2.07947073 | 0.0099158649 | 10.03827  | 0.2011597 | 5.64073545 |          |
| 7  | 5.507004  | 100.2938  | 2.07947066 | 0.0099158240 | 10.03827  | 0.2011597 | 5.64073526 |          |
| 8  | 5.506887  | 100.2939  | 2.07947057 | 0.0099157979 | 10.03827  | 0.2011597 | 5.64073503 |          |
| 9  | 5.506798  | 100.2940  | 2.07947047 | 0.0099157803 | 10.03827  | 0.2011597 | 5.64073480 |          |
| 10 | 5.506731  | 100.2940  | 2.07947038 | 0.0099157679 | 10.03827  | 0.2011597 | 5.64073459 |          |
| 11 | 5.506680  | 100.2940  | 2.28741717 | 0.0109073343 | 11.04210  | 0.2212756 | 6.20480751 |          |
| 12 | 5.892293  | 100.2964  | 1.94777009 | 0.0097388588 | 11.04159  | 0.2176911 | 5.43010828 |          |
| 13 | 6.367465  | 100.3094  | 1.63206298 | 0.0083899672 | 11.04152  | 0.2139888 | 4.68409586 |          |
| 14 | 7.064251  | 100.3355  | 1.33298550 | 0.0069455471 | 11.04224  | 0.2100283 | 3.95368964 |          |
| 15 | 8.049989  | 100.3720  | 1.04794440 | 0.0055158961 | 11.04350  | 0.2055896 | 3.23255868 |          |
| 16 | 9.339791  | 100.4134  | 0.77757745 | 0.0041621493 | 11.04501  | 0.2003279 | 2.51924133 |          |
| 17 | 10.921117 | 100.4519  | 0.52562418 | 0.0029066098 | 11.04652  | 0.1936400 | 1.81763375 |          |
| 18 | 12.746632 | 100.4782  | 0.30060551 | 0.0017695386 | 11.04768  | 0.1843230 | 1.14214749 |          |
| 19 | 14.684303 | 100.4820  | 0.12176395 | 0.0008156937 | 11.04784  | 0.1697361 | 0.53972378 |          |
| 20 | 16.447373 | 100.4567  | 0.03023479 | 0.0002523724 | 11.04619  | 0.1491231 | 0.17020863 |          |
| 21 | 18.787414 | 100.4118  | 0.01522386 | 0.0001382641 | 11.04728  | 0.1414420 | 0.09615844 |          |
|    | aprt      | arna      | asuc       | asli         | dada      | den       | dgnuc      |          |
| 1  | 0.9963412 | 1985.621  | 8.003186   | 8.003185     | 0.2004510 | 2.386351  | 0.1008502  |          |
| 2  | 0.9981831 | 1985.621  | 8.003012   | 8.003012     | 0.2004511 | 2.402707  | 0.1008503  |          |
| 3  | 0.9981332 | 1985.621  | 8.003028   | 8.003027     | 0.2004512 | 2.402833  | 0.1008504  |          |
| 4  | 0.9981052 | 1985.622  | 8.003042   | 8.003041     | 0.2004512 | 2.402879  | 0.1008504  |          |

|    |           |          |           |             |           |            |           |
|----|-----------|----------|-----------|-------------|-----------|------------|-----------|
| 5  | 0.9980919 | 1985.622 | 8.003053  | 8.003053    | 0.2004512 | 2.402911   | 0.1008504 |
| 6  | 0.9980853 | 1985.622 | 8.003064  | 8.003063    | 0.2004512 | 2.402935   | 0.1008504 |
| 7  | 0.9980816 | 1985.622 | 8.003072  | 8.003072    | 0.2004512 | 2.402953   | 0.1008504 |
| 8  | 0.9980795 | 1985.622 | 8.003080  | 8.003080    | 0.2004512 | 2.402967   | 0.1008504 |
| 9  | 0.9980783 | 1985.622 | 8.003087  | 8.003087    | 0.2004513 | 2.402977   | 0.1008504 |
| 10 | 0.9980775 | 1985.622 | 8.003093  | 8.003093    | 0.2004513 | 2.402985   | 0.1008504 |
| 11 | 1.0978846 | 2184.185 | 8.803409  | 8.803409    | 0.2204964 | 2.643290   | 0.1109354 |
| 12 | 1.0660070 | 2173.664 | 9.186490  | 9.207377    | 0.2204399 | 2.660299   | 0.1109561 |
| 13 | 1.0386327 | 2172.109 | 9.673546  | 9.693799    | 0.2202685 | 3.119270   | 0.1110638 |
| 14 | 0.9852818 | 2173.695 | 10.275909 | 10.296405   | 0.2199535 | 3.763921   | 0.1112884 |
| 15 | 0.9175062 | 2174.525 | 11.030531 | 11.051698   | 0.2194628 | 4.699088   | 0.1116437 |
| 16 | 0.8430669 | 2171.337 | 12.022671 | 12.044843   | 0.2187660 | 6.155691   | 0.1121430 |
| 17 | 0.7624260 | 2160.053 | 13.442904 | 13.465722   | 0.2178266 | 8.678945   | 0.1128056 |
| 18 | 0.6698860 | 2133.287 | 15.779704 | 15.802348   | 0.2165890 | 13.820582  | 0.1136629 |
| 19 | 0.5545486 | 2074.276 | 20.629994 | 20.650762   | 0.2149506 | 27.528781  | 0.1147714 |
| 20 | 0.4155372 | 1973.614 | 32.743065 | 32.750652   | 0.2127414 | 71.998777  | 0.1162378 |
| 21 | 0.3490630 | 1948.005 | 47.037441 | 47.038307   | 0.2100987 | 111.817126 | 0.1181374 |
|    | dnaa      | dnag     | gdna      | gdrnr       | gmp       | gmps       | gnuc      |
| 1  | 10.03756  | 6.826370 | 6.825859  | 0.1003440   | 0.5138721 | 1.5957628  | 4.807078  |
| 2  | 10.03756  | 6.826370 | 6.825863  | 0.1003438   | 0.5138758 | 1.5957629  | 4.807071  |
| 3  | 10.03756  | 6.826371 | 6.825864  | 0.1003439   | 0.5138768 | 1.5957629  | 4.807085  |
| 4  | 10.03756  | 6.826371 | 6.825864  | 0.1003440   | 0.5138774 | 1.5957628  | 4.807093  |
| 5  | 10.03756  | 6.826371 | 6.825865  | 0.1003440   | 0.5138776 | 1.5957627  | 4.807097  |
| 6  | 10.03756  | 6.826371 | 6.825865  | 0.1003440   | 0.5138777 | 1.5957626  | 4.807099  |
| 7  | 10.03756  | 6.826372 | 6.825865  | 0.1003440   | 0.5138778 | 1.5957625  | 4.807100  |
| 8  | 10.03756  | 6.826372 | 6.825866  | 0.1003440   | 0.5138777 | 1.5957624  | 4.807100  |
| 9  | 10.03756  | 6.826372 | 6.825866  | 0.1003440   | 0.5138777 | 1.5957623  | 4.807101  |
| 10 | 10.03756  | 6.826372 | 6.825866  | 0.1003440   | 0.5138777 | 1.5957622  | 4.807101  |
| 11 | 11.04132  | 7.509010 | 7.508453  | 0.1103784   | 0.5652655 | 1.7553383  | 5.287811  |
| 12 | 11.04132  | 7.509010 | 7.508106  | 0.1115850   | 0.5885785 | 1.7174249  | 5.415894  |
| 13 | 11.04132  | 7.509009 | 7.508058  | 0.1145702   | 0.6300674 | 1.6773472  | 5.740188  |
| 14 | 11.04132  | 7.509008 | 7.508551  | 0.1186844   | 0.6855959 | 1.6333970  | 6.201440  |
| 15 | 11.04132  | 7.509010 | 7.509405  | 0.1236232   | 0.7541371 | 1.5835068  | 6.775281  |
| 16 | 11.04133  | 7.509016 | 7.510433  | 0.1292989   | 0.8371371 | 1.5246584  | 7.460412  |
| 17 | 11.04134  | 7.509025 | 7.511460  | 0.1357848   | 0.9389181 | 1.4517185  | 8.275391  |
| 18 | 11.04136  | 7.509038 | 7.512250  | 0.1433395   | 1.0690032 | 1.3546662  | 9.266173  |
| 19 | 11.04138  | 7.509052 | 7.512353  | 0.1525608   | 1.2490797 | 1.2122299  | 10.534606 |
| 20 | 11.04140  | 7.509064 | 7.511233  | 0.1644974   | 1.4935988 | 1.0223255  | 12.273114 |
| 21 | 11.04142  | 7.509075 | 7.511978  | 0.1777200   | 1.6420994 | 0.9422041  | 14.322641 |
|    | grna      | gua      | hp        | hx          | hxd       | impd       | inuc      |
| 1  | 1323.532  | 1.154277 | 3.669760  | 0.047309283 | 1.1912809 | 1.595762   | 2.642505  |
| 2  | 1323.532  | 1.154508 | 3.684109  | 0.047320340 | 1.1914425 | 1.595750   | 2.642393  |
| 3  | 1323.532  | 1.154452 | 3.684104  | 0.047317303 | 1.1913981 | 1.595751   | 2.642401  |
| 4  | 1323.533  | 1.154411 | 3.684049  | 0.047314824 | 1.1913619 | 1.595751   | 2.642409  |
| 5  | 1323.533  | 1.154381 | 3.684001  | 0.047312868 | 1.1913333 | 1.595752   | 2.642416  |
| 6  | 1323.533  | 1.154359 | 3.683961  | 0.047311346 | 1.1913111 | 1.595753   | 2.642422  |
|    |           |          |           |             |           |            | mat       |



|    |            |           |           |             |           |           |          |           |
|----|------------|-----------|-----------|-------------|-----------|-----------|----------|-----------|
| 7  | 1323.533   | 1.154342  | 3.683929  | 0.047310172 | 1.1912939 | 1.595754  | 2.642427 | 14.988496 |
| 8  | 1323.533   | 1.154330  | 3.683904  | 0.047309277 | 1.1912809 | 1.595754  | 2.642432 | 14.988496 |
| 9  | 1323.533   | 1.154320  | 3.683883  | 0.047308602 | 1.1912710 | 1.595755  | 2.642437 | 14.988496 |
| 10 | 1323.533   | 1.154313  | 3.683868  | 0.047308101 | 1.1912637 | 1.595755  | 2.642441 | 14.988496 |
| 11 | 1191.180   | 1.038877  | 3.315469  | 0.042576963 | 1.0721325 | 1.436180  | 2.378200 | 13.489646 |
| 12 | 1185.442   | 1.074636  | 3.332793  | 0.044217209 | 1.0959128 | 1.435267  | 2.366367 | 13.239500 |
| 13 | 1184.594   | 1.117127  | 3.571861  | 0.043091721 | 1.0796362 | 1.431192  | 2.342745 | 13.047255 |
| 14 | 1185.459   | 1.176664  | 3.791614  | 0.039338661 | 1.0240242 | 1.425055  | 2.310857 | 12.830948 |
| 15 | 1185.911   | 1.256079  | 3.972777  | 0.033415831 | 0.9314979 | 1.417428  | 2.272680 | 12.575758 |
| 16 | 1184.173   | 1.352969  | 4.088332  | 0.025922163 | 0.8038583 | 1.408822  | 2.231642 | 12.262692 |
| 17 | 1178.019   | 1.463029  | 4.087727  | 0.017681229 | 0.6437957 | 1.400068  | 2.195027 | 11.858015 |
| 18 | 1163.422   | 1.580582  | 3.879544  | 0.009879505 | 0.4592477 | 1.393223  | 2.181401 | 11.293274 |
| 19 | 1131.239   | 1.696469  | 3.370087  | 0.004135197 | 0.2770341 | 1.395026  | 2.251939 | 10.420625 |
| 20 | 1076.342   | 1.795426  | 2.842668  | 0.001863272 | 0.1744223 | 1.430415  | 2.660277 | 9.330593  |
| 21 | 1062.375   | 1.918902  | 2.949563  | 0.003056118 | 0.2324434 | 1.507258  | 3.650163 | 9.073412  |
|    | polyam     | prpps     | pyr       | rnaa        | rnag      | trans     | ua       |           |
| 1  | 1.0079912  | 20.88492  | 9.999890  | 1985.551    | 1323.605  | 13.980504 | 2.314825 |           |
| 2  | 1.0079911  | 20.88278  | 10.043336 | 1985.551    | 1323.605  | 13.980503 | 2.314828 |           |
| 3  | 1.0079913  | 20.88275  | 10.043676 | 1985.551    | 1323.605  | 13.980504 | 2.314834 |           |
| 4  | 1.0079913  | 20.88274  | 10.043802 | 1985.550    | 1323.605  | 13.980504 | 2.314842 |           |
| 5  | 1.0079914  | 20.88274  | 10.043890 | 1985.550    | 1323.605  | 13.980504 | 2.314850 |           |
| 6  | 1.0079914  | 20.88273  | 10.043956 | 1985.550    | 1323.605  | 13.980505 | 2.314858 |           |
| 7  | 1.0079914  | 20.88273  | 10.044005 | 1985.550    | 1323.605  | 13.980504 | 2.314864 |           |
| 8  | 1.0079913  | 20.88273  | 10.044043 | 1985.550    | 1323.605  | 13.980504 | 2.314870 |           |
| 9  | 1.0079913  | 20.88273  | 10.044071 | 1985.550    | 1323.605  | 13.980504 | 2.314874 |           |
| 10 | 1.0079913  | 20.88273  | 10.044093 | 1985.550    | 1323.605  | 13.980504 | 2.314877 |           |
| 11 | 0.9071922  | 18.79445  | 9.039698  | 1786.995    | 1191.244  | 12.582454 | 2.083391 |           |
| 12 | 0.8877747  | 20.23712  | 8.868735  | 1809.912    | 1206.521  | 12.483028 | 2.083497 |           |
| 13 | 0.8591690  | 21.86937  | 9.605979  | 1830.077    | 1219.963  | 12.334014 | 2.084094 |           |
| 14 | 0.8275229  | 23.88575  | 10.578286 | 1848.292    | 1232.106  | 12.165453 | 2.085294 |           |
| 15 | 0.7916830  | 26.53032  | 11.846522 | 1864.846    | 1243.141  | 11.969548 | 2.086972 |           |
| 16 | 0.7497095  | 30.24237  | 13.563449 | 1879.681    | 1253.030  | 11.732837 | 2.088873 |           |
| 17 | 0.6984821  | 35.95754  | 16.042940 | 1892.424    | 1261.525  | 11.432272 | 2.090646 |           |
| 18 | 0.6322492  | 46.12503  | 19.983725 | 1902.238    | 1268.067  | 11.022192 | 2.091854 |           |
| 19 | 0.5393770  | 69.24126  | 27.226679 | 1907.322    | 1271.456  | 10.398472 | 2.092030 |           |
| 20 | 0.4137635  | 129.97672 | 41.107658 | 1904.248    | 1269.407  | 9.435207  | 2.090866 |           |
| 21 | 0.3489801  | 176.61601 | 50.415425 | 1895.156    | 1263.346  | 8.864125  | 2.088798 |           |
|    | x          | xd        | R5P       | Pi          |           |           |          |           |
| 1  | 0.03071716 | 2.314841  | 18        | 1400        |           |           |          |           |
| 2  | 0.03072109 | 2.314923  | 18        | 1400        |           |           |          |           |
| 3  | 0.03072380 | 2.314979  | 18        | 1400        |           |           |          |           |
| 4  | 0.03072494 | 2.315002  | 18        | 1400        |           |           |          |           |
| 5  | 0.03072508 | 2.315005  | 18        | 1400        |           |           |          |           |
| 6  | 0.03072464 | 2.314996  | 18        | 1400        |           |           |          |           |
| 7  | 0.03072389 | 2.314980  | 18        | 1400        |           |           |          |           |
| 8  | 0.03072300 | 2.314962  | 18        | 1400        |           |           |          |           |

```

9  0.03072209 2.314943 18 1400
10 0.03072121 2.314925 18 1400
11 0.02764837 2.083418 18 1400
12 0.02797124 2.090080 18 1400
13 0.02864558 2.103817 18 1400
14 0.02932191 2.117362 18 1400
15 0.02981142 2.127024 18 1400
16 0.02997677 2.130262 18 1400
17 0.02969569 2.124750 18 1400
18 0.02887989 2.108536 18 1400
19 0.02756496 2.081687 18 1400
20 0.02615075 2.051754 18 1400
21 0.02585287 2.045300 18 1400

```

Clearly, this system has stability sensitivity problems.

The folate model of Morrison and Allegra (JBC 1989) can be simulated as follows

```

> morr=readSBML(file.path(system.file(package="SBMLR"), "models/morrison.xml"))
> out1=sim(morr,seq(-20,0,1))
> morr$species$EMTX$ic=1 # bolus of methotrexate to 1 uM
> out2=sim(morr,0:30)
> outs=data.frame(rbind(out1,out2))
> attach(outs)
> par(mfrow=c(3,4))
> plot(time,FH2b,type="l",xlab="Hours")
> plot(time,FH2f,type="l",xlab="Hours")
> plot(time,DHFRf,type="l",xlab="Hours")
> plot(time,DHFRtot,type="l",xlab="Hours")
> plot(time,CHOFH4,type="l",xlab="Hours")
> plot(time,FH4,type="l",xlab="Hours")
> plot(time,CH2FH4,type="l",xlab="Hours")
> plot(time,CH3FH4,type="l",xlab="Hours")
> plot(time,AICARsyn,type="l",xlab="Hours")
> plot(time,MTR,type="l",xlab="Hours")
> plot(time,TYMS,type="l",xlab="Hours")
> #plot(time,EMTX,type="l",xlab="Hours")
> plot(time,DHFRductase,type="l",xlab="Hours")
> par(mfrow=c(1,1))
> detach(outs)

```

As final outputs in this document, the full curto summary and object are:

```
> summary(curto)
```

```

$Species
[1] 18

```

```

$sIDs
[1] "PRPP" "IMP" "SAMP" "ATP" "SAM" "Ade" "XMP" "GTP" "dATP" "dGTP"
[11] "RNA" "DNA" "HX" "Xa" "Gua" "UA" "R5P" "Pi"

$S0
      PRPP      IMP      SAMP      ATP      SAM      Ade
5.00000e+00 9.82634e+01 1.98189e-01 2.47535e+03 3.99187e+00 9.84730e-01
      XMP      GTP      dATP      dGTP      RNA      DNA
2.47930e+01 4.10223e+02 6.01413e+00 3.02581e+00 2.86805e+04 5.17934e+03
      HX      Xa      Gua      UA      R5P      Pi
9.51785e+00 5.05941e+00 5.50638e+00 1.00293e+02 1.80000e+01 1.40000e+03

$BC
PRPP  IMP  SAMP  ATP  SAM  Ade  XMP  GTP  dATP  dGTP  RNA  DNA  HX
FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
  Xa  Gua  UA  R5P  Pi
FALSE FALSE FALSE TRUE TRUE

$nStates
[1] 16

$y0
      PRPP      IMP      SAMP      ATP      SAM      Ade
5.00000e+00 9.82634e+01 1.98189e-01 2.47535e+03 3.99187e+00 9.84730e-01
      XMP      GTP      dATP      dGTP      RNA      DNA
2.47930e+01 4.10223e+02 6.01413e+00 3.02581e+00 2.86805e+04 5.17934e+03
      HX      Xa      Gua      UA
9.51785e+00 5.05941e+00 5.50638e+00 1.00293e+02

$nReactions
[1] 37

$rIDs
[1] "ada" "ade" "adna" "adrnr" "ampd" "aprt" "arna" "asuc"
[9] "asli" "dada" "den" "dgnuc" "dnaa" "dnag" "gdna" "gdrnr"
[17] "gmpr" "gmps" "gnuc" "gprr" "grna" "gua" "hprt" "hx"
[25] "hxd" "impd" "inuc" "mat" "polyam" "prpps" "pyr" "rnaa"
[33] "rnag" "trans" "ua" "x" "xd"

$rLaws
                                     ada
                                     "aada*ATP^fada4"
                                     ade
                                     "aade*Ade^fade6"
                                     adna

```

"aadna\*dATP^fdnap9\*dGTP^fdnap10"  
 adrnr  
 "aadrnr\*ATP^fadrnr4\*dATP^fadrnr9\*dGTP^fadrnr10"  
 ampd  
 "aampd\*ATP^fampd4\*GTP^fampd8\*Pi^fampd18"  
 aprt  
 "aaprt\*PRPP^faprt1\*ATP^faprt4\*Ade^faprt6"  
 arna  
 "aarna\*ATP^frnap4\*GTP^frnap8"  
 asuc  
 "aasuc\*IMP^fasuc2\*ATP^fasuc4\*GTP^fasuc8\*Pi^fasuc18"  
 asli  
 "aasli\*SAMP^fasli3\*ATP^fasli4"  
 dada  
 "adada\*dATP^fdada9"  
 den  
 "aden\*PRPP^fden1\*IMP^fden2\*ATP^fden4\*GTP^fden8\*Pi^fden18"  
 dgnuc  
 "adgnuc\*dGTP^fdgnuc10"  
 dnaa  
 "adnaa\*DNA^fdnan12"  
 dnag  
 "adnag\*DNA^fdnan12"  
 gdna  
 "agdna\*dATP^fdnap9\*dGTP^fdnap10"  
 gdrnr  
 "agdrnr\*GTP^fgdrnr8\*dATP^fgdrnr9\*dGTP^fgdrnr10"  
 gmpr  
 "agmpr\*IMP^fgmpr2\*ATP^fgmpr4\*XMP^fgmpr7\*GTP^fgmpr8"  
 gmps  
 "agmps\*ATP^fgmps4\*XMP^fgmps7"  
 gnuc  
 "agnuc\*GTP^fgnuc8\*Pi^fgnuc18"  
 gprr  
 "agprr\*PRPP^fgprr1\*GTP^fgprr8\*Gua^fgprr15"  
 grna  
 "agrna\*ATP^frnap4\*GTP^frnap8"  
 gua  
 "agua\*Gua^fgua15"  
 hprr  
 "ahprr\*PRPP^fhprr1\*IMP^fhprr2\*HX^fhprr13"  
 hx  
 "ahx\*HX^fhx13"  
 hxd  
 "ahxd\*HX^fhxd13"  
 impd

```

"aimpd*IMP^fimpd2*XMP^fimpd7*GTP^fimpd8"
      inuc
"ainuc*IMP^finuc2*Pi^finuc18"
      mat
"amat*ATP^fmat4*SAM^fmat5"
      polyam
"apolyam*SAM^fpolyam5"
      prpps
"aprpps*PRPP^fprpps1*ATP^fprpps4*GTP^fprpps8*R5P^fprpps17*Pi^fprpps18"
      pyr
"apyr*PRPP^fpyr1"
      rnaa
"arnaa*RNA^frnan11"
      rnag
"arnag*RNA^frnan11"
      trans
"atrans*SAM^ftrans5"
      ua
"aua*UA^fua16"
      x
"ax*Xa^fx14"
      xd
"axd*Xa^fxd14"

```

\$V0

|  | ada          | ade          | adna         | adrnr        | ampd         | aprt         |
|--|--------------|--------------|--------------|--------------|--------------|--------------|
|  | 2.079467e+00 | 9.915724e-03 | 1.003826e+01 | 2.011595e-01 | 5.640728e+00 | 9.963412e-01 |
|  | arna         | asuc         | asli         | dada         | den          | dgnuc        |
|  | 1.985621e+03 | 8.003186e+00 | 8.003185e+00 | 2.004510e-01 | 2.386351e+00 | 1.008502e-01 |
|  | dnaa         | dnag         | gdna         | gdrnr        | gmpr         | gmps         |
|  | 1.003756e+01 | 6.826370e+00 | 6.825859e+00 | 1.003440e-01 | 5.138721e-01 | 1.595763e+00 |
|  | gnuc         | gprrt        | grna         | gua          | hprrt        | hx           |
|  | 4.807078e+00 | 3.738009e+00 | 1.323532e+03 | 1.154277e+00 | 3.669760e+00 | 4.730928e-02 |
|  | hxd          | impd         | inuc         | mat          | polyam       | prpps        |
|  | 1.191281e+00 | 1.595762e+00 | 2.642505e+00 | 1.498849e+01 | 1.007991e+00 | 2.088492e+01 |
|  | pyr          | rnaa         | rnag         | trans        | ua           | x            |
|  | 9.999890e+00 | 1.985551e+03 | 1.323605e+03 | 1.398050e+01 | 2.314825e+00 | 3.071716e-02 |
|  | xd           |              |              |              |              |              |
|  | 2.314841e+00 |              |              |              |              |              |

\$globalVec

NULL

\$incid

|      | [,1] | [,2] | [,3] | [,4] | [,5] | [,6] | [,7] | [,8] | [,9] | [,10] | [,11] | [,12] | [,13] | [,14] |
|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|
| PRPP | 0    | 0    | 0    | 0    | 0    | -1   | 0    | 0    | 0    | 0     | -1    | 0     | 0     | 0     |

|      |       |       |       |       |       |       |       |       |       |       |       |       |    |    |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|----|----|
| IMP  | 0     | 0     | 0     | 0     | 1     | 0     | 0     | -1    | 0     | 0     | 1     | 0     | 0  | 0  |
| SAMP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 1     | -1    | 0     | 0     | 0     | 0  | 0  |
| ATP  | -1    | 0     | 0     | -1    | -1    | 1     | -1    | 0     | 1     | 0     | 0     | 0     | 0  | 0  |
| SAM  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
| Ade  | 0     | -1    | 0     | 0     | 0     | -1    | 0     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
| XMP  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
| GTP  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
| dATP | 0     | 0     | -1    | 1     | 0     | 0     | 0     | 0     | 0     | -1    | 0     | 0     | 1  | 0  |
| dGTP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | -1    | 0  | 1  |
| RNA  | 0     | 0     | 0     | 0     | 0     | 0     | 1     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
| DNA  | 0     | 0     | 1     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | -1 | -1 |
| HX   | 1     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 1     | 0     | 0     | 0  | 0  |
| Xa   | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
| Gua  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 1     | 0  | 0  |
| UA   | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  | 0  |
|      | [,15] | [,16] | [,17] | [,18] | [,19] | [,20] | [,21] | [,22] | [,23] | [,24] | [,25] | [,26] |    |    |
| PRPP | 0     | 0     | 0     | 0     | 0     | -1    | 0     | 0     | -1    | 0     | 0     | 0     | 0  |    |
| IMP  | 0     | 0     | 1     | 0     | 0     | 0     | 0     | 0     | 1     | 0     | 0     | -1    |    |    |
| SAMP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| ATP  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| SAM  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| Ade  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| XMP  | 0     | 0     | 0     | -1    | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 1  |    |
| GTP  | 0     | -1    | -1    | 1     | -1    | 1     | -1    | 0     | 0     | 0     | 0     | 0     | 0  |    |
| dATP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  |    |
| dGTP | -1    | 1     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  |    |
| RNA  | 0     | 0     | 0     | 0     | 0     | 0     | 1     | 0     | 0     | 0     | 0     | 0     | 0  |    |
| DNA  | 1     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0  |    |
| HX   | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | -1    | -1    | -1    | 0     |    |    |
| Xa   | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 1     | 0     | 0     | 1     | 0     |    |    |
| Gua  | 0     | 0     | 0     | 0     | 1     | -1    | 0     | -1    | 0     | 0     | 0     | 0     |    |    |
| UA   | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
|      | [,27] | [,28] | [,29] | [,30] | [,31] | [,32] | [,33] | [,34] | [,35] | [,36] | [,37] |       |    |    |
| PRPP | 0     | 0     | 0     | 1     | -1    | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| IMP  | -1    | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| SAMP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| ATP  | 0     | -1    | 0     | 0     | 0     | 1     | 0     | 1     | 0     | 0     | 0     | 0     |    |    |
| SAM  | 0     | 1     | -1    | 0     | 0     | 0     | 0     | -1    | 0     | 0     | 0     | 0     |    |    |
| Ade  | 0     | 0     | 1     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| XMP  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| GTP  | 0     | 0     | 0     | 0     | 0     | 0     | 1     | 0     | 0     | 0     | 0     | 0     |    |    |
| dATP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| dGTP | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| RNA  | 0     | 0     | 0     | 0     | 0     | -1    | -1    | 0     | 0     | 0     | 0     | 0     |    |    |
| DNA  | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |
| HX   | 1     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     | 0     |    |    |

|     |   |   |   |   |   |   |   |   |    |    |    |
|-----|---|---|---|---|---|---|---|---|----|----|----|
| Xa  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0  | -1 | -1 |
| Gua | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0  | 0  | 0  |
| UA  | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -1 | 0  | 1  |

\$nRules

[1] 0

\$ruleIDs

NULL

\$species

|      | index | initialConcentrations | boundaryConditions |
|------|-------|-----------------------|--------------------|
| PRPP | 1     | 5.00000e+00           | FALSE              |
| IMP  | 2     | 9.82634e+01           | FALSE              |
| SAMP | 3     | 1.98189e-01           | FALSE              |
| ATP  | 4     | 2.47535e+03           | FALSE              |
| SAM  | 5     | 3.99187e+00           | FALSE              |
| Ade  | 6     | 9.84730e-01           | FALSE              |
| XMP  | 7     | 2.47930e+01           | FALSE              |
| GTP  | 8     | 4.10223e+02           | FALSE              |
| dATP | 9     | 6.01413e+00           | FALSE              |
| dGTP | 10    | 3.02581e+00           | FALSE              |
| RNA  | 11    | 2.86805e+04           | FALSE              |
| DNA  | 12    | 5.17934e+03           | FALSE              |
| HX   | 13    | 9.51785e+00           | FALSE              |
| Xa   | 14    | 5.05941e+00           | FALSE              |
| Gua  | 15    | 5.50638e+00           | FALSE              |
| UA   | 16    | 1.00293e+02           | FALSE              |
| R5P  | 17    | 1.80000e+01           | TRUE               |
| Pi   | 18    | 1.40000e+03           | TRUE               |

\$reactions

|       | index |
|-------|-------|
| ada   | 1     |
| ade   | 2     |
| adna  | 3     |
| adrnr | 4     |
| ampd  | 5     |
| aprt  | 6     |
| arna  | 7     |
| asuc  | 8     |
| asli  | 9     |
| dada  | 10    |
| den   | 11    |
| dgnuc | 12    |
| dnaa  | 13    |

|        |    |
|--------|----|
| dnag   | 14 |
| gdna   | 15 |
| gdrnr  | 16 |
| gmpr   | 17 |
| gmpr   | 18 |
| gnuc   | 19 |
| gprt   | 20 |
| grna   | 21 |
| gua    | 22 |
| hprt   | 23 |
| hx     | 24 |
| hxd    | 25 |
| impd   | 26 |
| inuc   | 27 |
| mat    | 28 |
| polyam | 29 |
| prpps  | 30 |
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| ua     | 35 |
| x      | 36 |
| xd     | 37 |

|       |  |
|-------|--|
|       | Laws   |
| ada   | aada*ATP^fada4   |
| ade   | aade*Ade^fade6   |
| adna  | aadna*dATP^fdnap9*dGTP^fdnap10                           |
| adrnr | aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10            |
| ampd  | aampd*ATP^fampd4*dGTP^fampd8*Pi^fampd18                  |
| aprt  | aaprt*PRPP^faprt1*ATP^faprt4*Ade^faprt6                  |
| arna  | aarna*ATP^frnap4*dGTP^frnap8                             |
| asuc  | aasuc*IMP^fasuc2*ATP^fasuc4*dGTP^fasuc8*Pi^fasuc18       |
| asli  | aasli*SAMP^fasli3*ATP^fasli4                             |
| dada  | adada*dATP^fdada9  |
| den   | aden*PRPP^fden1*IMP^fden2*ATP^fden4*dGTP^fden8*Pi^fden18 |
| dgnuc | adgnuc*dGTP^fdgnuc10                                     |
| dnaa  | adnaa*DNA^fdnan12  |
| dnag  | adnag*DNA^fdnan12  |
| gdna  | agdna*dATP^fdnap9*dGTP^fdnap10                           |
| gdrnr | agdrnr*dGTP^fgdrnr8*dATP^fgdrnr9*dGTP^fgdrnr10           |
| gmpr  | agmpr*IMP^fgmpr2*ATP^fgmpr4*XMP^fgmpr7*dGTP^fgmpr8       |
| gmpr  | agmps*ATP^fgmps4*XMP^fgmps7                              |
| gnuc  | agnuc*dGTP^fgnuc8*Pi^fgnuc18                             |
| gprt  | agprt*PRPP^fgprt1*dGTP^fgprt8*Gua^fgprt15                |
| grna  | agrna*ATP^frnap4*dGTP^frnap8                             |



|        |   |  |
|--------|---|--|
| gua    |   | agua*Gua <sup>fgua15</sup>   |
| hprt   |   | ahprt*PRPP <sup>fhprt1</sup> *IMP <sup>fhprt2</sup> *HX <sup>fhprt13</sup> |
| hx     |   | ahx*HX <sup>fhx13</sup>  |
| hxd    |   | ahxd*HX <sup>fhxd13</sup>  |
| impd   |   | aimpd*IMP <sup>fimpd2</sup> *XMP <sup>fimpd7</sup> *GTP <sup>fimpd8</sup>  |
| inuc   |   | ainuc*IMP <sup>finuc2</sup> *Pi <sup>finuc18</sup>                         |
| mat    |   | amat*ATP <sup>fmat4</sup> *SAM <sup>fmat5</sup>                            |
| polyam |   | apolyam*SAM <sup>fpolyam5</sup>  |
| prpps  | aprpps*PRPP <sup>fprpps1</sup> *ATP <sup>fprpps4</sup> *GTP <sup>fprpps8</sup> *R5P <sup>fprpps17</sup> *Pi <sup>fprpps18</sup> |  |
| pyr    |   | apyr*PRPP <sup>fpyr1</sup>   |
| rnaa   |   | arnaa*RNA <sup>frnan11</sup>   |
| rnag   |   | arnag*RNA <sup>frnan11</sup>   |
| trans  |   | atrans*SAM <sup>ftrans5</sup>  |
| ua     |   | aua*UA <sup>fua16</sup>  |
| x      |   | ax*Xa <sup>fx14</sup>  |
| xd     |   | axd*Xa <sup>fxd14</sup>  |
|        | initialFluxes   |  |
| ada    | 2.079467e+00  |  |
| ade    | 9.915724e-03  |  |
| adna   | 1.003826e+01  |  |
| adrnr  | 2.011595e-01  |  |
| ampd   | 5.640728e+00  |  |
| aprt   | 9.963412e-01  |  |
| arna   | 1.985621e+03  |  |
| asuc   | 8.003186e+00  |  |
| asli   | 8.003185e+00  |  |
| dada   | 2.004510e-01  |  |
| den    | 2.386351e+00  |  |
| dgnuc  | 1.008502e-01  |  |
| dnaa   | 1.003756e+01  |  |
| dnag   | 6.826370e+00  |  |
| gdna   | 6.825859e+00  |  |
| gdrnr  | 1.003440e-01  |  |
| gmpr   | 5.138721e-01  |  |
| gmps   | 1.595763e+00  |  |
| gnuc   | 4.807078e+00  |  |
| gprt   | 3.738009e+00  |  |
| grna   | 1.323532e+03  |  |
| gua    | 1.154277e+00  |  |
| hprt   | 3.669760e+00  |  |
| hx     | 4.730928e-02  |  |
| hxd    | 1.191281e+00  |  |
| impd   | 1.595762e+00  |  |
| inuc   | 2.642505e+00  |  |
| mat    | 1.498849e+01  |  |
| polyam | 1.007991e+00  |  |

```

prpps  2.088492e+01
pyr    9.999890e+00
rnaa   1.985551e+03
rnag   1.323605e+03
trans  1.398050e+01
ua     2.314825e+00
x      3.071716e-02
xd     2.314841e+00

```

```
> curto
```

```
$sbml
```

```

                                xmlns
"http://www.sbml.org/sbml/level2"
                                level
                                "2"
                                version
                                "1"

```

```
$id
```

```
[1] "curto"
```

```
$notes
```

```

[1] "This is a purine metabolism model that is geared toward studies of gout."
[2] "The model is fully described in Curto et al., MBSC 151 (1998) pp 1-49"
[3] "The model uses Generalized Mass Action (GMA;i.e. power law) descriptions of reaction ra
[4] "Such descriptions are local approximations that assume independent substrate binding."
[5] "The de novo purine flux vden= 2.39 is in umole/min/KG, i.e. 2.4*60=144 uM/h if we let e
[6] "liter of water. Morrison and Allegra (JBC, 1989) have vden at 650 uM/h (model) and 415
[7] "The IC's below have been set to the system's steady state."
[8] "The units in this model are micromolar(uM) and minutes."
[9] "A cell volume of 1 is used so that amounts and concentrations are the same thing."

```

```
$compartments
```

```
$compartments$cell
```

```
$compartments$cell$id
```

```
[1] "cell"
```

```
$compartments$cell$size
```

```
[1] 1
```

```
$compartments$cell$name
```

```
[1] "cell"
```

```
$species
```

```
$species$PRPP
```

```

$species$PRPP$id
[1] "PRPP"

$species$PRPP$ic
[1] 5

$species$PRPP$compartment
[1] "cell"

$species$PRPP$bc
[1] FALSE

$species$IMP
$species$IMP$id
[1] "IMP"

$species$IMP$ic
[1] 98.2634

$species$IMP$compartment
[1] "cell"

$species$IMP$bc
[1] FALSE

$species$SAMP
$species$SAMP$id
[1] "SAMP"

$species$SAMP$ic
[1] 0.198189

$species$SAMP$compartment
[1] "cell"

$species$SAMP$bc
[1] FALSE

$species$ATP
$species$ATP$id
[1] "ATP"

$species$ATP$ic

```

```
[1] 2475.35
```

```
$species$ATP$compartment
```

```
[1] "cell"
```

```
$species$ATP$bc
```

```
[1] FALSE
```

```
$species$SAM
```

```
$species$SAM$id
```

```
[1] "SAM"
```

```
$species$SAM$ic
```

```
[1] 3.99187
```

```
$species$SAM$compartment
```

```
[1] "cell"
```

```
$species$SAM$bc
```

```
[1] FALSE
```

```
$species$Ade
```

```
$species$Ade$id
```

```
[1] "Ade"
```

```
$species$Ade$ic
```

```
[1] 0.98473
```

```
$species$Ade$compartment
```

```
[1] "cell"
```

```
$species$Ade$bc
```

```
[1] FALSE
```

```
$species$XMP
```

```
$species$XMP$id
```

```
[1] "XMP"
```

```
$species$XMP$ic
```

```
[1] 24.793
```

```
$species$XMP$compartment
```

```
[1] "cell"
```

```
$species$XMP$bc  
[1] FALSE
```

```
$species$GTP  
$species$GTP$id  
[1] "GTP"
```

```
$species$GTP$ic  
[1] 410.223
```

```
$species$GTP$compartment  
[1] "cell"
```

```
$species$GTP$bc  
[1] FALSE
```

```
$species$dATP  
$species$dATP$id  
[1] "dATP"
```

```
$species$dATP$ic  
[1] 6.01413
```

```
$species$dATP$compartment  
[1] "cell"
```

```
$species$dATP$bc  
[1] FALSE
```

```
$species$dGTP  
$species$dGTP$id  
[1] "dGTP"
```

```
$species$dGTP$ic  
[1] 3.02581
```

```
$species$dGTP$compartment  
[1] "cell"
```

```
$species$dGTP$bc  
[1] FALSE
```

```

$species$RNA
$species$RNA$id
[1] "RNA"

$species$RNA$ic
[1] 28680.5

$species$RNA$compartment
[1] "cell"

$species$RNA$bc
[1] FALSE

$species$DNA
$species$DNA$id
[1] "DNA"

$species$DNA$ic
[1] 5179.34

$species$DNA$compartment
[1] "cell"

$species$DNA$bc
[1] FALSE

$species$HX
$species$HX$id
[1] "HX"

$species$HX$ic
[1] 9.51785

$species$HX$compartment
[1] "cell"

$species$HX$bc
[1] FALSE

$species$Xa
$species$Xa$id
[1] "Xa"

```

```
$species$Xa$ic
```

```
[1] 5.05941
```

```
$species$Xa$compartment
```

```
[1] "cell"
```

```
$species$Xa$bc
```

```
[1] FALSE
```

```
$species$Gua
```

```
$species$Gua$id
```

```
[1] "Gua"
```

```
$species$Gua$ic
```

```
[1] 5.50638
```

```
$species$Gua$compartment
```

```
[1] "cell"
```

```
$species$Gua$bc
```

```
[1] FALSE
```

```
$species$UA
```

```
$species$UA$id
```

```
[1] "UA"
```

```
$species$UA$ic
```

```
[1] 100.293
```

```
$species$UA$compartment
```

```
[1] "cell"
```

```
$species$UA$bc
```

```
[1] FALSE
```

```
$species$R5P
```

```
$species$R5P$id
```

```
[1] "R5P"
```

```
$species$R5P$ic
```

```
[1] 18
```

```
$species$R5P$compartment  
[1] "cell"
```

```
$species$R5P$bc  
[1] TRUE
```

```
$species$Pi  
$species$Pi$id  
[1] "Pi"
```

```
$species$Pi$ic  
[1] 1400
```

```
$species$Pi$compartment  
[1] "cell"
```

```
$species$Pi$bc  
[1] TRUE
```

```
$globalParameters  
list()
```

```
$rules  
list()
```

```
$reactions  
$reactions$ada  
$reactions$ada$id  
[1] "ada"
```

```
$reactions$ada$reversible  
[1] FALSE
```

```
$reactions$ada$reactants  
[1] "ATP"
```

```
$reactions$ada$products  
[1] "HX"
```

```
$reactions$ada$parameters  
aada fada4  
0.001062 0.970000
```



```

$reactions$aada$mathmlLaw
<apply>
  <times/>
  <ci>aada</ci>
  <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fada4</ci>
  </apply>
</apply>

$reactions$aada$exprLaw
aada * ATP^fada4

$reactions$aada$strLaw
[1] "aada*ATP^fada4"

$reactions$aada$law
function (r, p = NULL)
{
  aada = p["aada"]
  fada4 = p["fada4"]
  ATP = r["ATP"]
  aada * ATP^fada4
}
<environment: 0x0000000005464610>

$reactions$ade
$reactions$ade$id
[1] "ade"

$reactions$ade$reversible
[1] FALSE

$reactions$ade$reactants
[1] "Ade"

$reactions$ade$parameters
aade fade6
0.01 0.55

$reactions$ade$mathmlLaw
<apply>
  <times/>
  <ci>aade</ci>

```

```

<apply>
  <power/>
  <ci>Ade</ci>
  <ci>fade6</ci>
</apply>
</apply>

$reactions$ade$exprLaw
aade * Ade^fade6

$reactions$ade$strLaw
[1] "aade*Ade^fade6"

$reactions$ade$law
function (r, p = NULL)
{
  aade = p["aade"]
  fade6 = p["fade6"]
  Ade = r["Ade"]
  aade * Ade^fade6
}
<environment: 0x000000000638afe0>

$reactions$adna
$reactions$adna$id
[1] "adna"

$reactions$adna$reversible
[1] FALSE

$reactions$adna$reactants
[1] "dATP"

$reactions$adna$modifiers
[1] "dGTP"

$reactions$adna$products
[1] "DNA"

$reactions$adna$parameters
  aadna  fdnap9 fdnap10
3.2789  0.4200  0.3300

$reactions$adna$mathmlLaw
<apply>

```

```

</times/>
<apply>
  <times/>
  <ci>aadna</ci>
  <apply>
    <power/>
    <ci>dATP</ci>
    <ci>fdnap9</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fdnap10</ci>
</apply>
</apply>

$reactions$adna$exprLaw
aadna * dATP^fdnap9 * dGTP^fdnap10

$reactions$adna$strLaw
[1] "aadna*dATP^fdnap9*dGTP^fdnap10"

$reactions$adna$law
function (r, p = NULL)
{
  aadna = p["aadna"]
  fdnap9 = p["fdnap9"]
  fdnap10 = p["fdnap10"]
  dATP = r["dATP"]
  dGTP = r["dGTP"]
  aadna * dATP^fdnap9 * dGTP^fdnap10
}
<environment: 0x000000005689740>

$reactions$adrnr
$reactions$adrnr$id
[1] "adrnr"

$reactions$adrnr$reversible
[1] FALSE

$reactions$adrnr$reactants
[1] "ATP"

```

```

$reactions$adnrn$modifiers
[1] "dGTP" "dATP"

$reactions$adnrn$products
[1] "dATP"

$reactions$adnrn$parameters
      aadnrn  fadnrn4  fadnrn9 fadnrn10
      0.0602   0.1000  -0.3000   0.8700

$reactions$adnrn$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>aadnrn</ci>
      <apply>
        <power/>
        <ci>ATP</ci>
        <ci>fadnrn4</ci>
      </apply>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>dATP</ci>
    <ci>fadnrn9</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fadnrn10</ci>
</apply>
</apply>

$reactions$adnrn$exprLaw
aadnrn * ATP^fadnrn4 * dATP^fadnrn9 * dGTP^fadnrn10

$reactions$adnrn$strLaw
[1] "aadnrn*ATP^fadnrn4*dATP^fadnrn9*dGTP^fadnrn10"

$reactions$adnrn$law
function (r, p = NULL)
{

```

```

aadrnr = p["aadrnr"]
fadrnr4 = p["fadrnr4"]
fadrnr9 = p["fadrnr9"]
fadrnr10 = p["fadrnr10"]
ATP = r["ATP"]
dGTP = r["dGTP"]
dATP = r["dATP"]
aadrnr * ATP^fadrnr4 * dATP^fadrnr9 * dGTP^fadrnr10
}
<environment: 0x000000000649eda8>

```

```

$reactions$ampd
$reactions$ampd$id
[1] "ampd"

$reactions$ampd$reversible
[1] FALSE

$reactions$ampd$reactants
[1] "ATP"

$reactions$ampd$modifiers
[1] "GTP" "Pi"

$reactions$ampd$products
[1] "IMP"

$reactions$ampd$parameters
  aampd  fampd4  fampd8  fampd18
0.02688 0.80000 -0.03000 -0.10000

$reactions$ampd$mathmlLaw
<apply>
<times/>
<apply>
<times/>
<apply>
<times/>
<ci>aampd</ci>
<apply>
<power/>
<ci>ATP</ci>
<ci>fampd4</ci>
</apply>
</apply>

```

```

    <apply>
      <power/>
      <ci>GTP</ci>
      <ci>fampd8</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>Pi</ci>
    <ci>fampd18</ci>
  </apply>
</apply>

$reactions$aampd$exprLaw
aampd * ATP^fampd4 * GTP^fampd8 * Pi^fampd18

$reactions$aampd$strLaw
[1] "aampd*ATP^fampd4*GTP^fampd8*Pi^fampd18"

$reactions$aampd$law
function (r, p = NULL)
{
  aampd = p["aampd"]
  fampd4 = p["fampd4"]
  fampd8 = p["fampd8"]
  fampd18 = p["fampd18"]
  ATP = r["ATP"]
  GTP = r["GTP"]
  Pi = r["Pi"]
  aampd * ATP^fampd4 * GTP^fampd8 * Pi^fampd18
}
<environment: 0x00000000056eaf90>

$reactions$aprt
$reactions$aprt$id
[1] "aprt"

$reactions$aprt$reversible
[1] FALSE

$reactions$aprt$reactants
[1] "PRPP" "Ade"

$reactions$aprt$modifiers
[1] "ATP"

```

```

$reactions$aprt$products
[1] "ATP"

$reactions$aprt$parameters
  aaprt faprt1 faprt4 faprt6
233.80  0.50 -0.80  0.75

$reactions$aprt$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>aaprt</ci>
      <apply>
        <power/>
        <ci>PRPP</ci>
        <ci>faprt1</ci>
      </apply>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>ATP</ci>
    <ci>faprt4</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>Ade</ci>
  <ci>faprt6</ci>
</apply>
</apply>

$reactions$aprt$exprLaw
aaprt * PRPP^faprt1 * ATP^faprt4 * Ade^faprt6

$reactions$aprt$strLaw
[1] "aaprt*PRPP^faprt1*ATP^faprt4*Ade^faprt6"

$reactions$aprt$law
function (r, p = NULL)
{
  aaprt = p["aaprt"]
  faprt1 = p["faprt1"]

```

```

    faprt4 = p["faprt4"]
    faprt6 = p["faprt6"]
    PRPP = r["PRPP"]
    Ade = r["Ade"]
    ATP = r["ATP"]
    aaprt * PRPP^faprt1 * ATP^faprt4 * Ade^faprt6
  }
<environment: 0x0000000005588268>

```

```

$reactions$arna
$reactions$arna$id
[1] "arna"

$reactions$arna$reversible
[1] FALSE

$reactions$arna$reactants
[1] "ATP"

$reactions$arna$modifiers
[1] "GTP"

$reactions$arna$products
[1] "RNA"

$reactions$arna$parameters
  aarna frnap4 frnap8
614.50  0.05  0.13

$reactions$arna$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>aarna</ci>
    <apply>
      <power/>
      <ci>ATP</ci>
      <ci>frnap4</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>frnap8</ci>

```



```

</apply>
</apply>

$reactions$aarna$exprLaw
aarna * ATP^frnap4 * GTP^frnap8

$reactions$aarna$strLaw
[1] "aarna*ATP^frnap4*GTP^frnap8"

$reactions$aarna$law
function (r, p = NULL)
{
  aarna = p["aarna"]
  frnap4 = p["frnap4"]
  frnap8 = p["frnap8"]
  ATP = r["ATP"]
  GTP = r["GTP"]
  aarna * ATP^frnap4 * GTP^frnap8
}
<environment: 0x000000004c7d830>

$reactions$asuc
$reactions$asuc$id
[1] "asuc"

$reactions$asuc$reversible
[1] FALSE

$reactions$asuc$reactants
[1] "IMP"

$reactions$asuc$modifiers
[1] "ATP" "GTP" "Pi"

$reactions$asuc$products
[1] "SAMP"

$reactions$asuc$parameters
  aasuc  fasuc2  fasuc4  fasuc8  fasuc18
3.5932  0.4000 -0.2400  0.2000 -0.0500

$reactions$asuc$mathmlLaw
<apply>
<times/>
<apply>

```

```

</times>
<apply>
  <times>
    <apply>
      <times>
        <ci>aasuc</ci>
        <apply>
          <power/>
          <ci>IMP</ci>
          <ci>fasuc2</ci>
        </apply>
      </apply>
    <apply>
      <power/>
      <ci>ATP</ci>
      <ci>fasuc4</ci>
    </apply>
  </apply>
<apply>
  <power/>
  <ci>GTP</ci>
  <ci>fasuc8</ci>
</apply>
</apply>
<apply>
  <power/>
  <ci>Pi</ci>
  <ci>fasuc18</ci>
</apply>
</apply>

$reactions$asuc$exprLaw
aasuc * IMP^fasuc2 * ATP^fasuc4 * GTP^fasuc8 * Pi^fasuc18

$reactions$asuc$strLaw
[1] "aasuc*IMP^fasuc2*ATP^fasuc4*GTP^fasuc8*Pi^fasuc18"

$reactions$asuc$law
function (r, p = NULL)
{
  aasuc = p["aasuc"]
  fasuc2 = p["fasuc2"]
  fasuc4 = p["fasuc4"]
  fasuc8 = p["fasuc8"]
  fasuc18 = p["fasuc18"]
  IMP = r["IMP"]

```

```

      ATP = r["ATP"]
      GTP = r["GTP"]
      Pi = r["Pi"]
      aasuc * IMP^fasuc2 * ATP^fasuc4 * GTP^fasuc8 * Pi^fasuc18
    }
<bytecode: 0x000000000801bba8>
<environment: 0x000000004be3490>

```

```

$reactions$asli
$reactions$asli$id
[1] "asli"

```

```

$reactions$asli$reversible
[1] FALSE

```

```

$reactions$asli$reactants
[1] "SAMP"

```

```

$reactions$asli$modifiers
[1] "ATP"

```

```

$reactions$asli$products
[1] "ATP"

```

```

$reactions$asli$parameters
      aasli  fasli3  fasli4
66544.00    0.99   -0.95

```

```

$reactions$asli$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>aasli</ci>
    <apply>
      <power/>
      <ci>SAMP</ci>
      <ci>fasli3</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fasli4</ci>
  </apply>

```

</apply>

```
$reactions$asli$exprLaw
aasli * SAMP^fasli3 * ATP^fasli4
```

```
$reactions$asli$strLaw
[1] "aasli*SAMP^fasli3*ATP^fasli4"
```

```
$reactions$asli$law
function (r, p = NULL)
{
  aasli = p["aasli"]
  fasli3 = p["fasli3"]
  fasli4 = p["fasli4"]
  SAMP = r["SAMP"]
  ATP = r["ATP"]
  aasli * SAMP^fasli3 * ATP^fasli4
}
<environment: 0x000000004b58890>
```

```
$reactions$dada
$reactions$dada$id
[1] "dada"
```

```
$reactions$dada$reversible
[1] FALSE
```

```
$reactions$dada$reactants
[1] "dATP"
```

```
$reactions$dada$products
[1] "HX"
```

```
$reactions$dada$parameters
  adada  fdada9
0.03333 1.00000
```

```
$reactions$dada$mathmlLaw
```

```
<apply>
  <times/>
  <ci>adada</ci>
  <apply>
    <power/>
    <ci>dATP</ci>
    <ci>fdada9</ci>
```

```

</apply>
</apply>

$reactions$dada$exprLaw
adada * dATP^fdada9

$reactions$dada$strLaw
[1] "adada*dATP^fdada9"

$reactions$dada$law
function (r, p = NULL)
{
  adada = p["adada"]
  fdada9 = p["fdada9"]
  dATP = r["dATP"]
  adada * dATP^fdada9
}
<environment: 0x0000000006565cd0>

$reactions$den
$reactions$den$id
[1] "den"

$reactions$den$reversible
[1] FALSE

$reactions$den$reactants
[1] "PRPP"

$reactions$den$modifiers
[1] "dGTP" "IMP" "ATP" "GTP" "Pi"

$reactions$den$products
[1] "IMP"

$reactions$den$parameters
      aden  fden1  fden2  fden4  fden8  fden18
5.2728  2.0000 -0.0600 -0.2500 -0.2000 -0.0800

$reactions$den$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>

```

```

</times>
<apply>
  <times>
    <apply>
      <times>
        <ci>aden</ci>
      <apply>
        <power>
          <ci>PRPP</ci>
          <ci>fden1</ci>
        </apply>
      </apply>
    </apply>
    <apply>
      <power>
        <ci>IMP</ci>
        <ci>fden2</ci>
      </apply>
    </apply>
    <apply>
      <power>
        <ci>ATP</ci>
        <ci>fden4</ci>
      </apply>
    </apply>
    <apply>
      <power>
        <ci>GTP</ci>
        <ci>fden8</ci>
      </apply>
    </apply>
    <apply>
      <power>
        <ci>Pi</ci>
        <ci>fden18</ci>
      </apply>
    </apply>
  </apply>

$reactions$den$exprLaw
aden * PRPP^fden1 * IMP^fden2 * ATP^fden4 * GTP^fden8 * Pi^fden18

$reactions$den$strLaw
[1] "aden*PRPP^fden1*IMP^fden2*ATP^fden4*GTP^fden8*Pi^fden18"

$reactions$den$law
function (r, p = NULL)
{

```

```

    aden = p["aden"]
    fden1 = p["fden1"]
    fden2 = p["fden2"]
    fden4 = p["fden4"]
    fden8 = p["fden8"]
    fden18 = p["fden18"]
    PRPP = r["PRPP"]
    dGTP = r["dGTP"]
    IMP = r["IMP"]
    ATP = r["ATP"]
    GTP = r["GTP"]
    Pi = r["Pi"]
    aden * PRPP^fden1 * IMP^fden2 * ATP^fden4 * GTP^fden8 * Pi^fden18
  }
<bytecode: 0x00000000086e7da8>
<environment: 0x000000000635b258>

$reactions$dgnuc
$reactions$dgnuc$id
[1] "dgnuc"

$reactions$dgnuc$reversible
[1] FALSE

$reactions$dgnuc$reactants
[1] "dGTP"

$reactions$dgnuc$products
[1] "Gua"

$reactions$dgnuc$parameters
  adg nuc fdg nuc10
0.03333 1.00000

$reactions$dgnuc$mathmlLaw
<apply>
  <times/>
  <ci>adg nuc</ci>
  <apply>
    <power/>
    <ci>dGTP</ci>
    <ci>fdg nuc10</ci>
  </apply>
</apply>

```

```

$reactions$dgnuc$exprLaw
adgnuc * dGTP^fdgnuc10

$reactions$dgnuc$strLaw
[1] "adgnuc*dGTP^fdgnuc10"

$reactions$dgnuc$law
function (r, p = NULL)
{
  adgnuc = p["adgnuc"]
  fdgnuc10 = p["fdgnuc10"]
  dGTP = r["dGTP"]
  adgnuc * dGTP^fdgnuc10
}
<environment: 0x000000004d007d0>

```

```

$reactions$dnaa
$reactions$dnaa$id
[1] "dnaa"

```

```

$reactions$dnaa$reversible
[1] FALSE

```

```

$reactions$dnaa$reactants
[1] "DNA"

```

```

$reactions$dnaa$products
[1] "dATP"

```

```

$reactions$dnaa$parameters
  adnaa fdnan12
0.001938 1.000000

```

```

$reactions$dnaa$mathmlLaw
<apply>
  <times/>
  <ci>adnaa</ci>
  <apply>
    <power/>
    <ci>DNA</ci>
    <ci>fdnan12</ci>
  </apply>
</apply>

```

```

$reactions$dnaa$exprLaw

```



```

adnaa * DNA^fdnan12

$reactions$dnaa$strLaw
[1] "adnaa * DNA^fdnan12"

$reactions$dnaa$law
function (r, p = NULL)
{
  adnaa = p["adnaa"]
  fdnan12 = p["fdnan12"]
  DNA = r["DNA"]
  adnaa * DNA^fdnan12
}
<environment: 0x00000000056d2da8>

$reactions$dnag
$reactions$dnag$id
[1] "dnag"

$reactions$dnag$reversible
[1] FALSE

$reactions$dnag$reactants
[1] "DNA"

$reactions$dnag$products
[1] "dGTP"

$reactions$dnag$parameters
  adnag  fdnan12
0.001318 1.000000

$reactions$dnag$mathmlLaw
<apply>
  <times/>
  <ci>adnag</ci>
  <apply>
    <power/>
    <ci>DNA</ci>
    <ci>fdnan12</ci>
  </apply>
</apply>

$reactions$dnag$exprLaw
adnag * DNA^fdnan12

```

```

$reactions$dnag$strLaw
[1] "adnag*DNA^fdnan12"

$reactions$dnag$law
function (r, p = NULL)
{
  adnag = p["adnag"]
  fdnan12 = p["fdnan12"]
  DNA = r["DNA"]
  adnag * DNA^fdnan12
}
<environment: 0x0000000004ebec20>

```

```

$reactions$gdna
$reactions$gdna$id
[1] "gdna"

```

```

$reactions$gdna$reversible
[1] FALSE

```

```

$reactions$gdna$reactants
[1] "dGTP"

```

```

$reactions$gdna$modifiers
[1] "dATP"

```

```

$reactions$gdna$products
[1] "DNA"

```

```

$reactions$gdna$parameters
  agdna  fdnap9 fdnap10
2.2296  0.4200  0.3300

```

```

$reactions$gdna$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>agdna</ci>
    <apply>
      <power/>
      <ci>dATP</ci>
      <ci>fdnap9</ci>
    </apply>
  </apply>

```

```

</apply>
<apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fdnap10</ci>
</apply>
</apply>

$reactions$gdna$exprLaw
agdna * dATP^fdnap9 * dGTP^fdnap10

$reactions$gdna$strLaw
[1] "agdna*dATP^fdnap9*dGTP^fdnap10"

$reactions$gdna$law
function (r, p = NULL)
{
  agdna = p["agdna"]
  fdnap9 = p["fdnap9"]
  fdnap10 = p["fdnap10"]
  dGTP = r["dGTP"]
  dATP = r["dATP"]
  agdna * dATP^fdnap9 * dGTP^fdnap10
}
<environment: 0x00000000064e2a30>

$reactions$gdrnr
$reactions$gdrnr$id
[1] "gdrnr"

$reactions$gdrnr$reversible
[1] FALSE

$reactions$gdrnr$reactants
[1] "GTP"

$reactions$gdrnr$modifiers
[1] "dATP" "dGTP"

$reactions$gdrnr$products
[1] "dGTP"

$reactions$gdrnr$parameters
  agdrnr  fgdrnr8  fgdrnr9 fgdrnr10
  0.1199   0.4000  -1.2000  -0.3900

```

```

$reactions$gdrnr$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>agdrnr</ci>
      <apply>
        <power/>
        <ci>GTP</ci>
        <ci>fgdrnr8</ci>
      </apply>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>dATP</ci>
    <ci>fgdrnr9</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fgdrnr10</ci>
</apply>
</apply>

$reactions$gdrnr$exprLaw
agdrnr * GTP^fgdrnr8 * dATP^fgdrnr9 * dGTP^fgdrnr10

$reactions$gdrnr$strLaw
[1] "agdrnr*GTP^fgdrnr8*dATP^fgdrnr9*dGTP^fgdrnr10"

$reactions$gdrnr$law
function (r, p = NULL)
{
  agdrnr = p["agdrnr"]
  fgdrnr8 = p["fgdrnr8"]
  fgdrnr9 = p["fgdrnr9"]
  fgdrnr10 = p["fgdrnr10"]
  GTP = r["GTP"]
  dATP = r["dATP"]
  dGTP = r["dGTP"]
  agdrnr * GTP^fgdrnr8 * dATP^fgdrnr9 * dGTP^fgdrnr10
}

```

```
<environment: 0x000000004ba4078>
```

```
$reactions$gmpr  
$reactions$gmpr$id  
[1] "gmpr"
```

```
$reactions$gmpr$reversible  
[1] FALSE
```

```
$reactions$gmpr$reactants  
[1] "GTP"
```

```
$reactions$gmpr$modifiers  
[1] "XMP" "ATP" "IMP"
```

```
$reactions$gmpr$products  
[1] "IMP"
```

```
$reactions$gmpr$parameters  
  agmpr fgmpr2 fgmpr4 fgmpr7 fgmpr8  
0.3005 -0.1500 -0.0700 -0.7600 0.7000
```

```
$reactions$gmpr$mathmlLaw
```

```
<apply>  
<times/>  
<apply>  
<times/>  
<apply>  
<times/>  
<apply>  
<times/>  
<ci>agmpr</ci>  
<apply>  
<power/>  
<ci>IMP</ci>  
<ci>fgmpr2</ci>  
</apply>  
</apply>  
<apply>  
<power/>  
<ci>ATP</ci>  
<ci>fgmpr4</ci>  
</apply>  
</apply>  
<apply>
```

```

    <power/>
    <ci>XMP</ci>
    <ci>fgmpr7</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>GTP</ci>
  <ci>fgmpr8</ci>
</apply>
</apply>

$reactions$gmpr$exprLaw
agmpr * IMP^fgmpr2 * ATP^fgmpr4 * XMP^fgmpr7 * GTP^fgmpr8

$reactions$gmpr$strLaw
[1] "agmpr*IMP^fgmpr2*ATP^fgmpr4*XMP^fgmpr7*GTP^fgmpr8"

$reactions$gmpr$law
function (r, p = NULL)
{
  agmpr = p["agmpr"]
  fgmpr2 = p["fgmpr2"]
  fgmpr4 = p["fgmpr4"]
  fgmpr7 = p["fgmpr7"]
  fgmpr8 = p["fgmpr8"]
  GTP = r["GTP"]
  XMP = r["XMP"]
  ATP = r["ATP"]
  IMP = r["IMP"]
  agmpr * IMP^fgmpr2 * ATP^fgmpr4 * XMP^fgmpr7 * GTP^fgmpr8
}
<bytecode: 0x0000000008ab6dd8>
<environment: 0x0000000005693b60>

$reactions$gmpr
$reactions$gmpr$id
[1] "gmpr"

$reactions$gmpr$reversible
[1] FALSE

$reactions$gmpr$reactants
[1] "XMP"

```

```

$reactions$gmps$modifiers
[1] "ATP"

$reactions$gmps$products
[1] "GTP"

$reactions$gmps$parameters
agmps fgmps4 fgmps7
0.3738 0.1200 0.1600

$reactions$gmps$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>agmps</ci>
    <apply>
      <power/>
      <ci>ATP</ci>
      <ci>fgmps4</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>XMP</ci>
    <ci>fgmps7</ci>
  </apply>
</apply>

$reactions$gmps$exprLaw
agmps * ATP^fgmps4 * XMP^fgmps7

$reactions$gmps$strLaw
[1] "agmps*ATP^fgmps4*XMP^fgmps7"

$reactions$gmps$law
function (r, p = NULL)
{
  agmps = p["agmps"]
  fgmps4 = p["fgmps4"]
  fgmps7 = p["fgmps7"]
  XMP = r["XMP"]
  ATP = r["ATP"]
  agmps * ATP^fgmps4 * XMP^fgmps7
}
<environment: 0x0000000051fdcc8>

```

```

$reactions$gnuc
$reactions$gnuc$id
[1] "gnuc"

$reactions$gnuc$reversible
[1] FALSE

$reactions$gnuc$reactants
[1] "GTP"

$reactions$gnuc$modifiers
[1] "Pi"

$reactions$gnuc$products
[1] "Gua"

$reactions$gnuc$parameters
  agnuc  fgnuc8 fgnuc18
0.2511  0.9000 -0.3400

$reactions$gnuc$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>agnuc</ci>
    <apply>
      <power/>
      <ci>GTP</ci>
      <ci>fgnuc8</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>Pi</ci>
    <ci>fgnuc18</ci>
  </apply>
</apply>

$reactions$gnuc$exprLaw
agnuc * GTP^fgnuc8 * Pi^fgnuc18

$reactions$gnuc$strLaw
[1] "agnuc*GTP^fgnuc8*Pi^fgnuc18"

```



```

$reactions$gnuc$law
function (r, p = NULL)
{
  agnuc = p["agnuc"]
  fgnuc8 = p["fgnuc8"]
  fgnuc18 = p["fgnuc18"]
  GTP = r["GTP"]
  Pi = r["Pi"]
  agnuc * GTP^fgnuc8 * Pi^fgnuc18
}
<environment: 0x00000000058dd780>

```

```

$reactions$gprt
$reactions$gprt$id
[1] "gprt"

```

```

$reactions$gprt$reversible
[1] FALSE

```

```

$reactions$gprt$reactants
[1] "Gua" "PRPP"

```

```

$reactions$gprt$modifiers
[1] "GTP"

```

```

$reactions$gprt$products
[1] "GTP"

```

```

$reactions$gprt$parameters
  agprt fgprt1 fgprt8 fgprt15
361.69   1.20  -1.20   0.42

```

```

$reactions$gprt$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>agprt</ci>
      <apply>
        <power/>
        <ci>PRPP</ci>
        <ci>fgprt1</ci>

```

```

    </apply>
  </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fgprt8</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>Gua</ci>
  <ci>fgprt15</ci>
</apply>
</apply>

$reactions$gpprt$exprLaw
agprt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15

$reactions$gpprt$strLaw
[1] "agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15"

$reactions$gpprt$law
function (r, p = NULL)
{
  agprt = p["agprt"]
  fgprt1 = p["fgprt1"]
  fgprt8 = p["fgprt8"]
  fgprt15 = p["fgprt15"]
  Gua = r["Gua"]
  PRPP = r["PRPP"]
  GTP = r["GTP"]
  agprt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15
}
<environment: 0x000000004fc5048>

$reactions$grna
$reactions$grna$id
[1] "grna"

$reactions$grna$reversible
[1] FALSE

$reactions$grna$reactants
[1] "GTP"

```

```

$reactions$grna$modifiers
[1] "ATP"

$reactions$grna$products
[1] "RNA"

$reactions$grna$parameters
agrna frnap4 frnap8
409.60 0.05 0.13

$reactions$grna$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>agrna</ci>
    <apply>
      <power/>
      <ci>ATP</ci>
      <ci>frnap4</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>frnap8</ci>
  </apply>
</apply>

$reactions$grna$exprLaw
agrna * ATP^frnap4 * GTP^frnap8

$reactions$grna$strLaw
[1] "agrna*ATP^frnap4*GTP^frnap8"

$reactions$grna$law
function (r, p = NULL)
{
  agrna = p["agrna"]
  frnap4 = p["frnap4"]
  frnap8 = p["frnap8"]
  GTP = r["GTP"]
  ATP = r["ATP"]
  agrna * ATP^frnap4 * GTP^frnap8
}
<environment: 0x0000000070bd918>

```

```

$reactions$gua
$reactions$gua$id
[1] "gua"

$reactions$gua$reversible
[1] FALSE

$reactions$gua$reactants
[1] "Gua"

$reactions$gua$products
[1] "Xa"

$reactions$gua$parameters
  agua fgua15
0.4919 0.5000

$reactions$gua$mathmlLaw
<apply>
  <times/>
  <ci>agua</ci>
  <apply>
    <power/>
    <ci>Gua</ci>
    <ci>fgua15</ci>
  </apply>
</apply>

$reactions$gua$exprLaw
agua * Gua^fgua15

$reactions$gua$strLaw
[1] "agua*Gua^fgua15"

$reactions$gua$law
function (r, p = NULL)
{
  agua = p["agua"]
  fgua15 = p["fgua15"]
  Gua = r["Gua"]
  agua * Gua^fgua15
}
<environment: 0x00000000070f2a38>

```

```

$reactions$hpert
$reactions$hpert$id
[1] "hpert"

$reactions$hpert$reversible
[1] FALSE

$reactions$hpert$reactants
[1] "HX"    "PRPP"

$reactions$hpert$modifiers
[1] "IMP"

$reactions$hpert$products
[1] "IMP"

$reactions$hpert$parameters
  ahprt  fhprt1  fhprt2 fhprt13
12.569   1.100  -0.890   0.480

$reactions$hpert$mathmlLaw
<apply>
<times/>
<apply>
<times/>
<apply>
<times/>
<ci>ahprt</ci>
<apply>
<power/>
<ci>PRPP</ci>
<ci>fhprt1</ci>
</apply>
</apply>
<apply>
<power/>
<ci>IMP</ci>
<ci>fhprt2</ci>
</apply>
</apply>
<apply>
<power/>
<ci>HX</ci>
<ci>fhprt13</ci>
</apply>

```

```

</apply>

$reactions$hpert$exprLaw
ahprt * PRPP^fhprt1 * IMP^fhprt2 * HX^fhprt13

$reactions$hpert$strLaw
[1] "ahprt*PRPP^fhprt1*IMP^fhprt2*HX^fhprt13"

$reactions$hpert$law
function (r, p = NULL)
{
  ahprt = p["ahprt"]
  fhprt1 = p["fhprt1"]
  fhprt2 = p["fhprt2"]
  fhprt13 = p["fhprt13"]
  HX = r["HX"]
  PRPP = r["PRPP"]
  IMP = r["IMP"]
  ahprt * PRPP^fhprt1 * IMP^fhprt2 * HX^fhprt13
}
<environment: 0x0000000007d0b2b0>

$reactions$hxx
$reactions$hxx$id
[1] "hxx"

$reactions$hxx$reversible
[1] FALSE

$reactions$hxx$reactants
[1] "HX"

$reactions$hxx$parameters
      ahx      fhx13
0.003793 1.120000

$reactions$hxx$mathmlLaw
<apply>
  <times/>
  <ci>ahx</ci>
  <apply>
    <power/>
    <ci>HX</ci>
    <ci>fhx13</ci>
  </apply>

```

```

</apply>

$reactions$h$x$exprLaw
ahx * HX^fhx13

$reactions$h$x$strLaw
[1] "ahx*HX^fhx13"

$reactions$h$x$law
function (r, p = NULL)
{
  ahx = p["ahx"]
  fhx13 = p["fhx13"]
  HX = r["HX"]
  ahx * HX^fhx13
}
<environment: 0x0000000007cbbda8>

$reactions$hxd
$reactions$hxd$id
[1] "hxd"

$reactions$hxd$reversible
[1] FALSE

$reactions$hxd$reactants
[1] "HX"

$reactions$hxd$products
[1] "Xa"

$reactions$hxd$parameters
  ahxd fhxd13
0.2754 0.6500

$reactions$hxd$mathmlLaw
<apply>
  <times/>
  <ci>ahxd</ci>
  <apply>
    <power/>
    <ci>HX</ci>
    <ci>fhxd13</ci>
  </apply>
</apply>

```

```

$reactions$hxd$exprLaw
ahxd * HX^fhxd13

$reactions$hxd$strLaw
[1] "ahxd*HX^fhxd13"

$reactions$hxd$law
function (r, p = NULL)
{
  ahxd = p["ahxd"]
  fhxd13 = p["fhxd13"]
  HX = r["HX"]
  ahxd * HX^fhxd13
}
<environment: 0x0000000007c78ad8>

```

```

$reactions$impd
$reactions$impd$id
[1] "impd"

$reactions$impd$reversible
[1] FALSE

$reactions$impd$reactants
[1] "IMP"

$reactions$impd$modifiers
[1] "GTP" "XMP"

$reactions$impd$products
[1] "XMP"

$reactions$impd$parameters
  aimpd fimpd2 fimpd7 fimpd8
1.2823 0.1500 -0.0900 -0.0300

$reactions$impd$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>aimpd</ci>

```



```

    <apply>
      <power/>
      <ci>IMP</ci>
      <ci>fimpd2</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>XMP</ci>
    <ci>fimpd7</ci>
  </apply>
</apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fimpd8</ci>
  </apply>
</apply>

$reactions$impd$exprLaw
aimpd * IMP^fimpd2 * XMP^fimpd7 * GTP^fimpd8

$reactions$impd$strLaw
[1] "aimpd*IMP^fimpd2*XMP^fimpd7*GTP^fimpd8"

$reactions$impd$law
function (r, p = NULL)
{
  aimpd = p["aimpd"]
  fimpd2 = p["fimpd2"]
  fimpd7 = p["fimpd7"]
  fimpd8 = p["fimpd8"]
  IMP = r["IMP"]
  GTP = r["GTP"]
  XMP = r["XMP"]
  aimpd * IMP^fimpd2 * XMP^fimpd7 * GTP^fimpd8
}
<environment: 0x000000007bc1408>

$reactions$inuc
$reactions$inuc$id
[1] "inuc"

$reactions$inuc$reversible
[1] FALSE

```

```

$reactions$inuc$reactants
[1] "IMP"

$reactions$inuc$modifiers
[1] "Pi"

$reactions$inuc$products
[1] "HX"

$reactions$inuc$parameters
  ainuc  finuc2 finuc18
0.9135  0.8000 -0.3600

$reactions$inuc$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>ainuc</ci>
    <apply>
      <power/>
      <ci>IMP</ci>
      <ci>finuc2</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>Pi</ci>
    <ci>finuc18</ci>
  </apply>
</apply>

$reactions$inuc$exprLaw
ainuc * IMP^finuc2 * Pi^finuc18

$reactions$inuc$strLaw
[1] "ainuc*IMP^finuc2*Pi^finuc18"

$reactions$inuc$law
function (r, p = NULL)
{
  ainuc = p["ainuc"]
  finuc2 = p["finuc2"]
  finuc18 = p["finuc18"]
  IMP = r["IMP"]

```

```

    Pi = r["Pi"]
    ainuc * IMP^finuc2 * Pi^finuc18
}
<environment: 0x000000000770d318>

```

```

$reactions$mat
$reactions$mat$id
[1] "mat"

```

```

$reactions$mat$reversible
[1] FALSE

```

```

$reactions$mat$reactants
[1] "ATP"

```

```

$reactions$mat$modifiers
[1] "SAM"

```

```

$reactions$mat$products
[1] "SAM"

```

```

$reactions$mat$parameters
      amat   fmat4   fmat5
7.2067  0.2000 -0.6000

```

```

$reactions$mat$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <ci>amat</ci>
    <apply>
      <power/>
      <ci>ATP</ci>
      <ci>fmat4</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>SAM</ci>
    <ci>fmat5</ci>
  </apply>
</apply>

```

```

$reactions$mat$exprLaw

```

```

amat * ATP^fmat4 * SAM^fmat5

$reactions$mat$strLaw
[1] "amat*ATP^fmat4*SAM^fmat5"

$reactions$mat$law
function (r, p = NULL)
{
  amat = p["amat"]
  fmat4 = p["fmat4"]
  fmat5 = p["fmat5"]
  ATP = r["ATP"]
  SAM = r["SAM"]
  amat * ATP^fmat4 * SAM^fmat5
}
<environment: 0x000000007693b20>

$reactions$polyam
$reactions$polyam$id
[1] "polyam"

$reactions$polyam$reversible
[1] FALSE

$reactions$polyam$reactants
[1] "SAM"

$reactions$polyam$products
[1] "Ade"

$reactions$polyam$parameters
apolyam fpolyam5
0.29      0.90

$reactions$polyam$mathmlLaw
<apply>
  <times/>
  <ci>apolyam</ci>
  <apply>
    <power/>
    <ci>SAM</ci>
    <ci>fpolyam5</ci>
  </apply>
</apply>

```

```

$reactions$polyam$exprLaw
apolyam * SAM^fpolyam5

$reactions$polyam$strLaw
[1] "apolyam*SAM^fpolyam5"

$reactions$polyam$law
function (r, p = NULL)
{
  apolyam = p["apolyam"]
  fpolyam5 = p["fpolyam5"]
  SAM = r["SAM"]
  apolyam * SAM^fpolyam5
}
<environment: 0x0000000076613a0>

$reactions$prpps
$reactions$prpps$id
[1] "prpps"

$reactions$prpps$reversible
[1] FALSE

$reactions$prpps$reactants
[1] "R5P"

$reactions$prpps$modifiers
[1] "ATP" "GTP" "Pi" "PRPP"

$reactions$prpps$products
[1] "PRPP"

$reactions$prpps$parameters
  aprpps fprpps1 fprpps4 fprpps8 fprpps17 fprpps18
    0.90   -0.03   -0.45   -0.04    0.65    0.70

$reactions$prpps$mathmlLaw
<apply>
<times/>
<apply>
<times/>
<apply>
<times/>
<apply>
<times/>

```

```

    <apply>
      <times/>
      <ci>aprpps</ci>
    </apply>
    <apply>
      <power/>
      <ci>PRPP</ci>
      <ci>fprpps1</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fprpps4</ci>
  </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fprpps8</ci>
  </apply>
  <apply>
    <power/>
    <ci>R5P</ci>
    <ci>fprpps17</ci>
  </apply>
  <apply>
    <power/>
    <ci>Pi</ci>
    <ci>fprpps18</ci>
  </apply>
</apply>

$reactions$prpps$exprLaw
aprpps * PRPP^fprpps1 * ATP^fprpps4 * GTP^fprpps8 * R5P^fprpps17 *
  Pi^fprpps18

$reactions$prpps$strLaw
[1] "aprpps*PRPP^fprpps1*ATP^fprpps4*GTP^fprpps8*R5P^fprpps17*Pi^fprpps18"

$reactions$prpps$law
function (r, p = NULL)
{
  aprpps = p["aprpps"]
  fprpps1 = p["fprpps1"]

```

```

fprpps4 = p["fprpps4"]
fprpps8 = p["fprpps8"]
fprpps17 = p["fprpps17"]
fprpps18 = p["fprpps18"]
R5P = r["R5P"]
ATP = r["ATP"]
GTP = r["GTP"]
Pi = r["Pi"]
PRPP = r["PRPP"]
aprpss * PRPP^fprpps1 * ATP^fprpps4 * GTP^fprpps8 * R5P^fprpps17 *
  Pi^fprpps18
}
<bytecode: 0x0000000008f0db18>
<environment: 0x00000000076045c8>

```

```

$reactions$pyr
$reactions$pyr$id
[1] "pyr"

```

```

$reactions$pyr$reversible
[1] FALSE

```

```

$reactions$pyr$reactants
[1] "PRPP"

```

```

$reactions$pyr$parameters
  apyr  fpyr1
1.2951 1.2700

```

```

$reactions$pyr$mathmlLaw
<apply>
  <times/>
  <ci>apyr</ci>
  <apply>
    <power/>
    <ci>PRPP</ci>
    <ci>fpyr1</ci>
  </apply>
</apply>

```

```

$reactions$pyr$exprLaw
apyr * PRPP^fpyr1

```

```

$reactions$pyr$strLaw
[1] "apyr*PRPP^fpyr1"

```

```

$reactions$pyr$law
function (r, p = NULL)
{
  apyr = p["apyr"]
  fpyr1 = p["fpyr1"]
  PRPP = r["PRPP"]
  apyr * PRPP^fpyr1
}
<environment: 0x00000000075c4e18>

```

```

$reactions$rnaa
$reactions$rnaa$id
[1] "rnaa"

```

```

$reactions$rnaa$reversible
[1] FALSE

```

```

$reactions$rnaa$reactants
[1] "RNA"

```

```

$reactions$rnaa$products
[1] "ATP"

```

```

$reactions$rnaa$parameters
  arnaa frnan11
0.06923 1.00000

```

```

$reactions$rnaa$mathmlLaw
<apply>
  <times/>
  <ci>arna</ci>
  <apply>
    <power/>
    <ci>RNA</ci>
    <ci>frnan11</ci>
  </apply>
</apply>

```

```

$reactions$rnaa$exprLaw
arna * RNA^frnan11

```

```

$reactions$rnaa$strLaw
[1] "arna*RNA^frnan11"

```



```

$reactions$rnaa$law
function (r, p = NULL)
{
  arnaa = p["arnaa"]
  frnan11 = p["frnan11"]
  RNA = r["RNA"]
  arnaa * RNA^frnan11
}
<environment: 0x00000000075961c8>

```

```

$reactions$rnag
$reactions$rnag$id
[1] "rnag"

```

```

$reactions$rnag$reversible
[1] FALSE

```

```

$reactions$rnag$reactants
[1] "RNA"

```

```

$reactions$rnag$products
[1] "GTP"

```

```

$reactions$rnag$parameters
  arnag frnan11
0.04615 1.00000

```

```

$reactions$rnag$mathmlLaw
<apply>
  <times/>
  <ci>arnag</ci>
  <apply>
    <power/>
    <ci>RNA</ci>
    <ci>frnan11</ci>
  </apply>
</apply>

```

```

$reactions$rnag$exprLaw
arnag * RNA^frnan11

```

```

$reactions$rnag$strLaw
[1] "arnag*RNA^frnan11"

```

```

$reactions$rnag$law

```

```

function (r, p = NULL)
{
  arnag = p["arnag"]
  frnan11 = p["frnan11"]
  RNA = r["RNA"]
  arnag * RNA^frnan11
}
<environment: 0x000000007559568>

```

```

$reactions$trans
$reactions$trans$id
[1] "trans"

```

```

$reactions$trans$reversible
[1] FALSE

```

```

$reactions$trans$reactants
[1] "SAM"

```

```

$reactions$trans$products
[1] "ATP"

```

```

$reactions$trans$parameters
  atrans ftrans5
8.8539 0.3300

```

```

$reactions$trans$mathmlLaw
<apply>
  <times/>
  <ci>atrans</ci>
  <apply>
    <power/>
    <ci>SAM</ci>
    <ci>ftrans5</ci>
  </apply>
</apply>

```

```

$reactions$trans$exprLaw
atrans * SAM^ftrans5

```

```

$reactions$trans$strLaw
[1] "atrans*SAM^ftrans5"

```

```

$reactions$trans$law
function (r, p = NULL)

```

```

{
  atrans = p["atrans"]
  ftrans5 = p["ftrans5"]
  SAM = r["SAM"]
  atrans * SAM^ftrans5
}
<environment: 0x0000000007487670>

```

```

$reactions$ua
$reactions$ua$id
[1] "ua"

```

```

$reactions$ua$reversible
[1] FALSE

```

```

$reactions$ua$reactants
[1] "UA"

```

```

$reactions$ua$parameters
      aua      fua16
8.744e-05 2.210e+00

```

```

$reactions$ua$mathmlLaw
<apply>
  <times/>
  <ci>aua</ci>
  <apply>
    <power/>
    <ci>UA</ci>
    <ci>fua16</ci>
  </apply>
</apply>

```

```

$reactions$ua$exprLaw
aua * UA^fua16

```

```

$reactions$ua$strLaw
[1] "aua*UA^fua16"

```

```

$reactions$ua$law
function (r, p = NULL)
{
  aua = p["aua"]
  fua16 = p["fua16"]
  UA = r["UA"]

```

```

    aua * UA^fua16
}
<environment: 0x00000000073c1c38>

$reactions$x
$reactions$x$id
[1] "x"

$reactions$x$reversible
[1] FALSE

$reactions$x$reactants
[1] "Xa"

$reactions$x$parameters
    ax    fx14
0.0012 2.0000

$reactions$x$mathmlLaw
<apply>
  <times/>
  <ci>ax</ci>
  <apply>
    <power/>
    <ci>Xa</ci>
    <ci>fx14</ci>
  </apply>
</apply>

$reactions$x$exprLaw
ax * Xa^fx14

$reactions$x$strLaw
[1] "ax*Xa^fx14"

$reactions$x$law
function (r, p = NULL)
{
  ax = p["ax"]
  fx14 = p["fx14"]
  Xa = r["Xa"]
  ax * Xa^fx14
}
<environment: 0x00000000073151d0>

```

```

$reactions$xd
$reactions$xd$id
[1] "xd"

$reactions$xd$reversible
[1] FALSE

$reactions$xd$reactants
[1] "Xa"

$reactions$xd$products
[1] "UA"

$reactions$xd$parameters
  axd fxd14
0.949 0.550

$reactions$xd$mathmlLaw
<apply>
  <times/>
  <ci>axd</ci>
  <apply>
    <power/>
    <ci>Xa</ci>
    <ci>fxd14</ci>
  </apply>
</apply>

$reactions$xd$exprLaw
axd * Xa^fxd14

$reactions$xd$strLaw
[1] "axd*Xa^fxd14"

$reactions$xd$law
function (r, p = NULL)
{
  axd = p["axd"]
  fxd14 = p["fxd14"]
  Xa = r["Xa"]
  axd * Xa^fxd14
}
<environment: 0x000000000714ac08>

```

```
$htmlNotes
```

```
<notes>
```

```
<body xmlns="http://www.w3.org/1999/xhtml">
```

```
<p>This is a purine metabolism model that is geared toward studies of gout.</p>
```

```
<p>The model is fully described in Curto et al., MBSC 151 (1998) pp 1-49</p>
```

```
<p>The model uses Generalized Mass Action (GMA;i.e. power law) descriptions of reaction ra
```

```
<p>Such descriptions are local approximations that assume independent substrate binding.</p>
```

```
<p/>
```

```
<p>The de novo purine flux vden= 2.39 is in umole/min/KG, i.e. 2.4*60=144 uM/h if we let e
```

```
<p>liter of water. Morrison and Allegra (JBC, 1989) have vden at 650 uM/h (model) and 415
```

```
<p>The IC&apos;s below have been set to the system&apos;s steady state.</p>
```

```
<p>The units in this model are micromolar(uM) and minutes.</p>
```

```
<p>A cell volume of 1 is used so that amounts and concentrations are the same thing.</p>
```

```
</body>
```

```
</notes>
```

```
attr("class")
```

```
[1] "SBMLR"
```