# Quick Intro to SBMLR

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## 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^fada4   2.079466999
ade       2                                 aade*Ade^fade6   0.009915724
adna      3                 aadna*dATP^fdnap9*dGTP^fdnap10  10.038261346
adrnr     4 aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10   0.201159500
ampd      5        aampd*ATP^fampd4*GTP^fampd8*Pi^fampd18   5.640727920
aprt      6       aaprt*PRPP^faprt1*ATP^faprt4*Ade^faprt6   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 multipied 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 | gmps | 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 bumples
```

```
   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 0.048063714  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 19.417928 167.86461 0.007564062   14.10886 1.380950 0.0003501154
        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 | 5.6407279 |
| 2 | 5.508591 | 100.2931 | 2.07946890 | 0.0099167492 | 10.03827 | 0.2011596 | 5.6407325 |
| 3 | 5.508056 | 100.2932 | 2.07947007 | 0.0099162922 | 10.03827 | 0.2011597 | 5.6407345 |
| 4 | 5.507660 | 100.2933 | 2.07947058 | 0.0099160532 | 10.03827 | 0.2011597 | 5.6407353 |
| 5 | 5.507373 | 100.2935 | 2.07947074 | 0.0099159315 | 10.03827 | 0.2011597 | 5.6407355 |
| 6 | 5.507162 | 100.2936 | 2.07947073 | 0.0099158649 | 10.03827 | 0.2011597 | 5.6407355 |
| 7 | 5.507004 | 100.2938 | 2.07947066 | 0.0099158240 | 10.03827 | 0.2011597 | 5.6407353 |
| 8 | 5.506887 | 100.2939 | 2.07947057 | 0.0099157979 | 10.03827 | 0.2011597 | 5.6407350 |
| 9 | 5.506798 | 100.2940 | 2.07947047 | 0.0099157803 | 10.03827 | 0.2011597 | 5.6407348 |
| 10 | 5.506731 | 100.2940 | 2.07947038 | 0.0099157679 | 10.03827 | 0.2011597 | 5.6407346 |
| 11 | 5.506680 | 100.2940 | 2.28741717 | 0.0109073343 | 11.04210 | 0.2212756 | 6.2048075 |
| 12 | 5.892293 | 100.2964 | 1.94777009 | 0.0097388588 | 11.04159 | 0.2176911 | 5.4301083 |
| 13 | 6.367465 | 100.3094 | 1.63206298 | 0.0083899672 | 11.04152 | 0.2139888 | 4.6840959 |
| 14 | 7.064251 | 100.3355 | 1.33298550 | 0.0069455471 | 11.04224 | 0.2100283 | 3.9536896 |
| 15 | 8.049989 | 100.3720 | 1.04794440 | 0.0055158961 | 11.04350 | 0.2055896 | 3.2325587 |
| 16 | 9.339791 | 100.4134 | 0.77757745 | 0.0041621493 | 11.04501 | 0.2003279 | 2.5192413 |
| 17 | 10.921117 | 100.4519 | 0.52562418 | 0.0029066098 | 11.04652 | 0.1936400 | 1.8176338 |
| 18 | 12.746632 | 100.4782 | 0.30060551 | 0.0017695386 | 11.04768 | 0.1843230 | 1.1421475 |
| 19 | 14.684303 | 100.4820 | 0.12176395 | 0.0008156937 | 11.04784 | 0.1697361 | 0.5397238 |
| 20 | 16.447373 | 100.4567 | 0.03023479 | 0.0002523724 | 11.04619 | 0.1491231 | 0.1702086 |
| 21 | 18.787414 | 100.4118 | 0.01522385 | 0.0001382639 | 11.04728 | 0.1414420 | 0.0961584 |

| | 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 | 0.3490627 | 1948.005 | 47.037446 | 47.038303 | 0.2100987 | 111.817157 | 0.1181374 |

| | dnaa | dnag | gdna | gdrnr | gmpr | gmps | gnuc | gprt |
|---|---|---|---|---|---|---|---|---|
| 1 | 10.03756 | 6.826370 | 6.825859 | 0.1003440 | 0.5138721 | 1.595763 | 4.807078 | 3.738009 |
| 2 | 10.03756 | 6.826370 | 6.825863 | 0.1003438 | 0.5138758 | 1.595763 | 4.807071 | 3.753992 |
| 3 | 10.03756 | 6.826371 | 6.825864 | 0.1003439 | 0.5138768 | 1.595763 | 4.807085 | 3.753944 |
| 4 | 10.03756 | 6.826371 | 6.825864 | 0.1003440 | 0.5138774 | 1.595763 | 4.807093 | 3.753867 |
| 5 | 10.03756 | 6.826371 | 6.825865 | 0.1003440 | 0.5138776 | 1.595763 | 4.807097 | 3.753812 |
| 6 | 10.03756 | 6.826371 | 6.825865 | 0.1003440 | 0.5138777 | 1.595763 | 4.807099 | 3.753773 |
| 7 | 10.03756 | 6.826372 | 6.825865 | 0.1003440 | 0.5138778 | 1.595762 | 4.807100 | 3.753744 |
| 8 | 10.03756 | 6.826372 | 6.825866 | 0.1003440 | 0.5138777 | 1.595762 | 4.807100 | 3.753723 |
| 9 | 10.03756 | 6.826372 | 6.825866 | 0.1003440 | 0.5138777 | 1.595762 | 4.807101 | 3.753708 |
| 10 | 10.03756 | 6.826372 | 6.825866 | 0.1003440 | 0.5138777 | 1.595762 | 4.807101 | 3.753696 |
| 11 | 11.04132 | 7.509010 | 7.508453 | 0.1103784 | 0.5652655 | 1.755338 | 5.287811 | 4.129056 |
| 12 | 11.04132 | 7.509010 | 7.508106 | 0.1115850 | 0.5885785 | 1.717425 | 5.415894 | 4.041125 |
| 13 | 11.04132 | 7.509009 | 7.508058 | 0.1145702 | 0.6300674 | 1.677347 | 5.740188 | 4.166225 |
| 14 | 11.04132 | 7.509008 | 7.508551 | 0.1186844 | 0.6855959 | 1.633397 | 6.201440 | 4.300262 |
| 15 | 11.04132 | 7.509010 | 7.509405 | 0.1236232 | 0.7541371 | 1.583507 | 6.775281 | 4.493036 |
| 16 | 11.04133 | 7.509016 | 7.510433 | 0.1292989 | 0.8371371 | 1.524658 | 7.460412 | 4.779762 |
| 17 | 11.04134 | 7.509025 | 7.511460 | 0.1357848 | 0.9389181 | 1.451719 | 8.275391 | 5.209518 |
| 18 | 11.04136 | 7.509038 | 7.512250 | 0.1433395 | 1.0690032 | 1.354666 | 9.266173 | 5.883606 |
| 19 | 11.04138 | 7.509052 | 7.512353 | 0.1525608 | 1.2490797 | 1.212230 | 10.534606 | 7.048233 |
| 20 | 11.04140 | 7.509064 | 7.511233 | 0.1644974 | 1.4935988 | 1.022326 | 12.273114 | 8.899788 |
| 21 | 11.04142 | 7.509075 | 7.511978 | 0.1777200 | 1.6420995 | 0.942204 | 14.322641 | 9.289103 |

| | grna | gua | hprt | hx | hxd | impd | inuc | mat |
|---|---|---|---|---|---|---|---|---|
| 1 | 1323.532 | 1.154277 | 3.669760 | 0.047309283 | 1.1912809 | 1.595762 | 2.642505 | 14.988492 |
| 2 | 1323.532 | 1.154508 | 3.684109 | 0.047320340 | 1.1914425 | 1.595750 | 2.642393 | 14.988495 |
| 3 | 1323.532 | 1.154452 | 3.684104 | 0.047317303 | 1.1913981 | 1.595751 | 2.642401 | 14.988496 |
| 4 | 1323.533 | 1.154411 | 3.684049 | 0.047314824 | 1.1913619 | 1.595751 | 2.642409 | 14.988496 |
| 5 | 1323.533 | 1.154381 | 3.684001 | 0.047312868 | 1.1913333 | 1.595752 | 2.642416 | 14.988496 |
| 6 | 1323.533 | 1.154359 | 3.683961 | 0.047311346 | 1.1913111 | 1.595753 | 2.642422 | 14.988496 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 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 | 9.073411 |

| | 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 | 176.61605 | 50.415430 | 1895.156 | 1263.346 | 8.864124 | 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,DHFReductase,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)

$nSpecies
[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 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"   "gprt"   "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"
gprt
"agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15"
grna
"agrna*ATP^frnap4*GTP^frnap8"
gua
"agua*Gua^fgua15"
hprt
"ahprt*PRPP^fhprt1*IMP^fhprt2*HX^fhprt13"
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         gprt         grna          gua         hprt           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 |
| 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 | 1 |
| GTP | 0 | -1 | -1 | 1 | -1 | 1 | -1 | 0 | 0 | 0 | 0 | 0 |
| dATP | 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 |
| RNA | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| DNA | 1 | 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 |
| IMP | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| SAMP | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| ATP | 0 | -1 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 0 |
| SAM | 0 | 1 | -1 | 0 | 0 | 0 | 0 | -1 | 0 | 0 | 0 |
| Ade | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| XMP | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| GTP | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| dATP | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| dGTP | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| RNA | 0 | 0 | 0 | 0 | 0 | -1 | -1 | 0 | 0 | 0 | 0 |
| DNA | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| HX | 1 | 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
gmps      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
pyr       31
rnaa      32
rnag      33
trans     34
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*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
gprt                                agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15
grna                                             agrna*ATP^frnap4*GTP^frnap8
```

```
gua                                                          agua*Gua^fgua15
hprt                                  ahprt*PRPP^fhprt1*IMP^fhprt2*HX^fhprt13
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
       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                              level
"http://www.sbml.org/sbml/level2"                                "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
```

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

$reactions$ada$exprLaw
aada * ATP^fada4

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

$reactions$ada$law
function (r, p = NULL)
{
    aada = p["aada"]
    fada4 = p["fada4"]
    ATP = r["ATP"]
    aada * ATP^fada4
}
<environment: 0x557bd7502cc0>


$reactions$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: 0x557bd755dc10>


$reactions$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: 0x557bd75905c8>


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

$reactions$adrnr$reversible
[1] FALSE

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

```
$reactions$adrnr$modifiers
[1] "dGTP" "dATP"

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

$reactions$adrnr$parameters
  aadrnr  fadrnr4  fadrnr9 fadrnr10
  0.0602   0.1000  -0.3000   0.8700

$reactions$adrnr$mathmlLaw
<apply>
 <times/>
 <apply>
  <times/>
  <apply>
   <times/>
   <ci>aadrnr</ci>
   <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fadrnr4</ci>
   </apply>
  </apply>
  <apply>
   <power/>
   <ci>dATP</ci>
   <ci>fadrnr9</ci>
  </apply>
 </apply>
 <apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fadrnr10</ci>
 </apply>
</apply>

$reactions$adrnr$exprLaw
aadrnr * ATP^fadrnr4 * dATP^fadrnr9 * dGTP^fadrnr10

$reactions$adrnr$strLaw
[1] "aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10"

$reactions$adrnr$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: 0x557bd75d3ff0>


$reactions$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>

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

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

$reactions$ampd$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: 0x557bd7615ba0>


$reactions$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>
   <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: 0x557bd765d930>


$reactions$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>

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

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

$reactions$arna$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: 0x557bd7697160>


$reactions$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: 0x557bd8c3d130>
<environment: 0x557bd76e2fe8>


$reactions$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: 0x557bd771e9c0>


$reactions$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: 0x557bd7746ff8>


$reactions$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>
     <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>

$reactions$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: 0x557bd620a910>
<environment: 0x557bd779b710>


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

$reactions$dgnuc$reversible
[1] FALSE

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

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

$reactions$dgnuc$parameters
  adgnuc fdgnuc10
 0.03333  1.00000

$reactions$dgnuc$mathmlLaw
<apply>
 <times/>
 <ci>adgnuc</ci>
 <apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fdgnuc10</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: 0x557bd77d5478>


$reactions$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: 0x557bd77fa7d0>


$reactions$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: 0x557bd781dce8>


$reactions$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>
  <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: 0x557bd78505c0>


$reactions$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>
   <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: 0x557bd7893448>


$reactions$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: 0x557bd5546d98>
<environment: 0x557bd78e0af8>


$reactions$gmps
$reactions$gmps$id
[1] "gmps"

$reactions$gmps$reversible
[1] FALSE

$reactions$gmps$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: 0x557bd791e710>
```

```
$reactions$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: 0x557bd7954178>


$reactions$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>

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

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

$reactions$gprt$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: 0x557bd7995070>


$reactions$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: 0x557bd79cdd70>
```

```
$reactions$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: 0x557bd79f4488>
```

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

$reactions$hprt$reversible
[1] FALSE

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

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

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

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

$reactions$hprt$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>

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

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

$reactions$hprt$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: 0x557bd7a39d90>


$reactions$hx
$reactions$hx$id
[1] "hx"

$reactions$hx$reversible
[1] FALSE

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

$reactions$hx$parameters
     ahx    fhx13
0.003793 1.120000

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

```
</apply>

$reactions$hx$exprLaw
ahx * HX^fhx13

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

$reactions$hx$law
function (r, p = NULL)
{
    ahx = p["ahx"]
    fhx13 = p["fhx13"]
    HX = r["HX"]
    ahx * HX^fhx13
}
<environment: 0x557bd7a65580>


$reactions$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: 0x557bd7a88a28>


$reactions$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: 0x557bd7ac6730>


$reactions$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: 0x557bd7aff350>


$reactions$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: 0x557bd7b36c58>


$reactions$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: 0x557bd7b5f290>


$reactions$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>
      <power/>
      <ci>PRPP</ci>
      <ci>fprpps1</ci>
     </apply>
    </apply>
    <apply>
     <power/>
     <ci>ATP</ci>
     <ci>fprpps4</ci>
    </apply>
   </apply>
   <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fprpps8</ci>
   </apply>
  </apply>
  <apply>
   <power/>
   <ci>R5P</ci>
   <ci>fprpps17</ci>
  </apply>
 </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"]
    aprpps * PRPP^fprpps1 * ATP^fprpps4 * GTP^fprpps8 * R5P^fprpps17 *
        Pi^fprpps18
}
<bytecode: 0x557bd390b2f0>
<environment: 0x557bd7bb5858>


$reactions$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: 0x557bd7be7128>


$reactions$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>arnaa</ci>
 <apply>
  <power/>
  <ci>RNA</ci>
  <ci>frnan11</ci>
 </apply>
</apply>

$reactions$rnaa$exprLaw
arnaa * RNA^frnan11

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

```
$reactions$rnaa$law
function (r, p = NULL)
{
    arnaa = p["arnaa"]
    frnan11 = p["frnan11"]
    RNA = r["RNA"]
    arnaa * RNA^frnan11
}
<environment: 0x557bd7c0e3a0>


$reactions$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: 0x557bd7c356f8>


$reactions$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: 0x557bd7c5aac0>


$reactions$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: 0x557bd7c7def8>


$reactions$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: 0x557bd7ca7090>
```

```
$reactions$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: 0x557bd7ccc458>
```

```
$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>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"
```