

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 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 | |

| | | | | | | | | |
|----|-----------|------------|-----------|----------|----------|------------|----------|----------|
| 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 | gmpr | gmpr | gnuc | gprt | |
| 1 | 10.03756 | 6.826370 | 6.825859 | 0.1003440 | 0.5138721 | 1.5957628 | 4.807078 | 3.738009 | |
| 2 | 10.03756 | 6.826370 | 6.825863 | 0.1003438 | 0.5138758 | 1.5957629 | 4.807071 | 3.753992 | |
| 3 | 10.03756 | 6.826371 | 6.825864 | 0.1003439 | 0.5138768 | 1.5957629 | 4.807085 | 3.753944 | |
| 4 | 10.03756 | 6.826371 | 6.825864 | 0.1003440 | 0.5138774 | 1.5957628 | 4.807093 | 3.753867 | |
| 5 | 10.03756 | 6.826371 | 6.825865 | 0.1003440 | 0.5138776 | 1.5957627 | 4.807097 | 3.753812 | |
| 6 | 10.03756 | 6.826371 | 6.825865 | 0.1003440 | 0.5138777 | 1.5957626 | 4.807099 | 3.753773 | |
| 7 | 10.03756 | 6.826372 | 6.825865 | 0.1003440 | 0.5138778 | 1.5957625 | 4.807100 | 3.753744 | |
| 8 | 10.03756 | 6.826372 | 6.825866 | 0.1003440 | 0.5138777 | 1.5957624 | 4.807100 | 3.753723 | |
| 9 | 10.03756 | 6.826372 | 6.825866 | 0.1003440 | 0.5138777 | 1.5957623 | 4.807101 | 3.753708 | |
| 10 | 10.03756 | 6.826372 | 6.825866 | 0.1003440 | 0.5138777 | 1.5957622 | 4.807101 | 3.753696 | |
| 11 | 11.04132 | 7.509010 | 7.508453 | 0.1103784 | 0.5652655 | 1.7553383 | 5.287811 | 4.129056 | |
| 12 | 11.04132 | 7.509010 | 7.508106 | 0.1115850 | 0.5885785 | 1.7174249 | 5.415894 | 4.041125 | |
| 13 | 11.04132 | 7.509009 | 7.508058 | 0.1145702 | 0.6300674 | 1.6773472 | 5.740188 | 4.166225 | |
| 14 | 11.04132 | 7.509008 | 7.508551 | 0.1186844 | 0.6855959 | 1.6333970 | 6.201440 | 4.300262 | |
| 15 | 11.04132 | 7.509010 | 7.509405 | 0.1236232 | 0.7541371 | 1.5835068 | 6.775281 | 4.493036 | |
| 16 | 11.04133 | 7.509016 | 7.510433 | 0.1292989 | 0.8371371 | 1.5246584 | 7.460412 | 4.779762 | |
| 17 | 11.04134 | 7.509025 | 7.511460 | 0.1357848 | 0.9389181 | 1.4517185 | 8.275391 | 5.209518 | |
| 18 | 11.04136 | 7.509038 | 7.512250 | 0.1433395 | 1.0690032 | 1.3546662 | 9.266173 | 5.883606 | |
| 19 | 11.04138 | 7.509052 | 7.512353 | 0.1525608 | 1.2490797 | 1.2122299 | 10.534606 | 7.048233 | |
| 20 | 11.04140 | 7.509064 | 7.511233 | 0.1644974 | 1.4935988 | 1.0223255 | 12.273114 | 8.899788 | |
| 21 | 11.04142 | 7.509075 | 7.511978 | 0.1777200 | 1.6420994 | 0.9422041 | 14.322641 | 9.289103 | |
| | grna | gua | hprr | 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 | 9.073412 |
| | 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,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" "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"
 adnr
 "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"
 gmpr
 "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      adrn      amp      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      gprr      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 | 0 | 0 |
| IMP | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | -1 | 0 |
| SAMP | 0 | 0 | 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 | 0 | 0 |
| SAM | 0 | 0 | 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 | 0 | 0 |
| XMP | 0 | 0 | 0 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| GTP | 0 | -1 | -1 | 1 | -1 | 1 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| dATP | 0 | 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 | 0 |
| RNA | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| DNA | 1 | 0 | 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 | 0 | 0 |
| Xa | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 |
| Gua | 0 | 0 | 0 | 0 | 1 | -1 | 0 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| UA | 0 | 0 | 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 | 0 | 0 |
| IMP | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| SAMP | 0 | 0 | 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 | 0 | 0 |
| SAM | 0 | 1 | -1 | 0 | 0 | 0 | 0 | -1 | 0 | 0 | 0 | 0 | 0 | 0 |
| Ade | 0 | 0 | 1 | 0 | 0 | 0 | 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 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| dATP | 0 | 0 | 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 | 0 | 0 |
| RNA | 0 | 0 | 0 | 0 | 0 | -1 | -1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| DNA | 0 | 0 | 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 | 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 |
| gprr | 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 |
| aprr | aaprr*PRPP^faprr1*ATP^faprr4*Ade^faprr6 |
| 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 ^f gua15 |
| hprt | | ahprt*PRPP ^f hprt1*IMP ^f hprt2*HX ^f hprt13 |
| hx | | ahx*HX ^f hx13 |
| hxd | | ahxd*HX ^f hxd13 |
| impd | | aimpd*IMP ^f fimpd2*XMP ^f fimpd7*GTP ^f fimpd8 |
| inuc | | ainuc*IMP ^f finuc2*Pi ^f finuc18 |
| mat | | amat*ATP ^f mat4*SAM ^f mat5 |
| polyam | | apolyam*SAM ^f polyam5 |
| prpps | aprpps*PRPP ^f fprpps1*ATP ^f fprpps4*GTP ^f fprpps8*R5P ^f fprpps17*Pi ^f fprpps18 | |
| pyr | | apyr*PRPP ^f fpyr1 |
| rnaa | | arnaa*RNA ^f frnan11 |
| rnag | | arnag*RNA ^f frnan11 |
| trans | | atrans*SAM ^f ftrans5 |
| ua | | aua*UA ^f fua16 |
| x | | ax*Xa ^f fx14 |
| xd | | axd*Xa ^f 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

```



```

$reactions$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: 0x4b5a4b8>

```

```

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

```

```

$reactions$aade$reversible
[1] FALSE

```

```

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

```

```

$reactions$aade$parameters
aade fade6
0.01 0.55

```

```

$reactions$aade$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: 0x48bb310>

$reactions$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: 0x53995e0>

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

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

$reactions$adnrn$strLaw
[1] "adnrn*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: 0x53ec680>

```

```

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

```

```

$reactions$aampd$reversible
[1] FALSE

```

```

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

```

```

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

```

```

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

```

```

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

```

```

$reactions$aampd$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>aampd</ci>
      <apply>
        <power/>
        <ci>ATP</ci>
        <ci>fampd4</ci>
      </apply>
    </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: 0x544d5d0>

```

```

$reactions$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: 0x54ac968>

```

```

$reactions$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
  arna 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: 0x54f4ff8>

$reactions$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>
    <power/>
    <ci>GTP</ci>
    <ci>fasuc8</ci>
  </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: 0x55ccda0>
<environment: 0x5557810>

```

```

$reactions$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: 0x55aa400>

$reactions$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: 0x55e2218>

$reactions$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: 0x4b3f9c8>
<environment: 0x564ec60>

```

```

$reactions$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: 0x5698140>

$reactions$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: 0x56c9ed8>

$reactions$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: 0x56f9fa0>

$reactions$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: 0x5739248>

$reactions$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: 0x57903a8>

\$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: 0x4cf63a0>
<environment: 0x58a2160>

$reactions$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: 0x58ea100>

```

```

$reactions$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: 0x5927930>

```

```

$reactions$gpprt
$reactions$gpprt$id
[1] "gpprt"

```

```

$reactions$gpprt$reversible
[1] FALSE

```

```

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

```

```

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

```

```

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

```

```

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

```

```

$reactions$gpprt$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: 0x51c5920>

```

```

$reactions$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: 0x5174c10>

```

```

$reactions$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: 0x51398f8>

```

```

$reactions$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: 0x50eb348>

$reactions$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>

```

```

</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: 0x50a03c0>

$reactions$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: 0x505add0>

$reactions$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: 0x4fad1e0>

```

```

$reactions$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: 0x4f5aeb8>

```

```

$reactions$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: 0x4f14020>

$reactions$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: 0x4eb1768>

$reactions$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"]
aprrps * PRPP^fprpps1 * ATP^fprpps4 * GTP^fprpps8 * R5P^fprpps17 *
  Pi^fprpps18
}
<bytecode: 0x5c94f18>
<environment: 0x4e106a8>

```

```

$reactions$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: 0x4da9df8>

```

```

$reactions$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: 0x4d58d98>

```

```

$reactions$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: 0x4d05a78>

```

```

$reactions$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: 0x4cc75f8>

```

```

$reactions$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: 0x4c7f7a8>

$reactions$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: 0x4c42550>

```

```

$reactions$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: 0x4bffb0>

```

```
$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"
```