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 conditions is a steady state. It then shows the time course response to an increase in [PRPP] from 5 uM to 50 uM.

```
> out1 = simulate(curto, seq(-20, 0, 1))
> curto$species$PRPP$ic = 50
> out2 = simulate(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 *simulate* is either NULL, a vector of numbers, or a list of interpolation functions (time varying enzyme concentration boundary conditions). The vector and list lengths 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
> simulate(curto, (-10):10, modulator = rep(2, 37))
```

```
      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 5.017095 98.25819 0.1981608 2475.352 3.991870 0.9849150 24.79299
 [3,]   -8 5.017228 98.25854 0.1981855 2475.354 3.991870 0.9848419 24.79298
 [4,]   -7 5.017271 98.25887 0.1981857 2475.354 3.991870 0.9848024 24.79296
 [5,]   -6 5.017300 98.25916 0.1981859 2475.354 3.991871 0.9847828 24.79295
 [6,]   -5 5.017320 98.25940 0.1981862 2475.354 3.991871 0.9847718 24.79295
 [7,]   -4 5.017340 98.25965 0.1981864 2475.354 3.991871 0.9847607 24.79294
 [8,]   -3 5.017356 98.25986 0.1981866 2475.354 3.991871 0.9847534 24.79293
 [9,]   -2 5.017367 98.26005 0.1981867 2475.354 3.991871 0.9847490 24.79292
[10,]   -1 5.017378 98.26024 0.1981869 2475.354 3.991871 0.9847446 24.79291
[11,]    0 5.017385 98.26043 0.1981870 2475.354 3.991870 0.9847418 24.79291
[12,]    1 5.017391 98.26063 0.1981872 2475.354 3.991870 0.9847403 24.79290
[13,]    2 5.017396 98.26082 0.1981873 2475.354 3.991870 0.9847388 24.79289
[14,]    3 5.017401 98.26101 0.1981875 2475.354 3.991870 0.9847373 24.79289
[15,]    4 5.017406 98.26121 0.1981877 2475.354 3.991870 0.9847358 24.79288
[16,]    5 5.017411 98.26140 0.1981878 2475.354 3.991870 0.9847343 24.79287
[17,]    6 5.017414 98.26154 0.1981879 2475.354 3.991870 0.9847336 24.79287
[18,]    7 5.017415 98.26166 0.1981880 2475.354 3.991870 0.9847333 24.79286
[19,]    8 5.017416 98.26177 0.1981881 2475.354 3.991870 0.9847330 24.79286
[20,]    9 5.017417 98.26188 0.1981882 2475.354 3.991870 0.9847327 24.79286
[21,]   10 5.017418 98.26199 0.1981883 2475.354 3.991870 0.9847325 24.79285
          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,] 410.2235 6.014136 3.025813 28680.49 5179.340 9.519325 5.059924 5.508098
 [4,] 410.2242 6.014137 3.025814 28680.49 5179.341 9.518915 5.059998 5.507735
 [5,] 410.2245 6.014137 3.025814 28680.49 5179.341 9.518635 5.059997 5.507502
 [6,] 410.2247 6.014138 3.025814 28680.49 5179.341 9.518427 5.059962 5.507337
 [7,] 410.2248 6.014138 3.025814 28680.49 5179.341 9.518219 5.059927 5.507171
 [8,] 410.2249 6.014139 3.025814 28680.49 5179.341 9.518064 5.059883 5.507048
 [9,] 410.2250 6.014139 3.025814 28680.49 5179.342 9.517952 5.059833 5.506960
[10,] 410.2251 6.014139 3.025814 28680.49 5179.342 9.517841 5.059783 5.506871
[11,] 410.2251 6.014140 3.025814 28680.49 5179.342 9.517771 5.059735 5.506809
[12,] 410.2251 6.014141 3.025814 28680.49 5179.343 9.517736 5.059691 5.506769
[13,] 410.2251 6.014142 3.025814 28680.49 5179.343 9.517701 5.059646 5.506728
[14,] 410.2251 6.014143 3.025815 28680.49 5179.343 9.517667 5.059601 5.506687
[15,] 410.2251 6.014143 3.025815 28680.49 5179.344 9.517632 5.059556 5.506647
[16,] 410.2251 6.014144 3.025815 28680.49 5179.344 9.517597 5.059512 5.506606
[17,] 410.2251 6.014145 3.025815 28680.49 5179.345 9.517588 5.059487 5.506585
[18,] 410.2251 6.014146 3.025815 28680.49 5179.345 9.517594 5.059475 5.506575
[19,] 410.2251 6.014147 3.025815 28680.49 5179.345 9.517601 5.059463 5.506566
[20,] 410.2251 6.014148 3.025815 28680.49 5179.346 9.517607 5.059451 5.506556
[21,] 410.2251 6.014149 3.025815 28680.49 5179.346 9.517613 5.059438 5.506547
           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 0.9981829
 [3,] 100.2932 2.079470 0.009916344 10.03827 0.2011597  5.640734 0.9981402
 [4,] 100.2933 2.079470 0.009916125 10.03827 0.2011597  5.640735 0.9981143
 [5,] 100.2935 2.079471 0.009916017 10.03827 0.2011597  5.640735 0.9981021
 [6,] 100.2936 2.079471 0.009915956 10.03827 0.2011597  5.640735 0.9980957
 [7,] 100.2937 2.079471 0.009915895 10.03827 0.2011597  5.640735 0.9980894
 [8,] 100.2937 2.079471 0.009915854 10.03827 0.2011597  5.640735 0.9980853
 [9,] 100.2938 2.079470 0.009915830 10.03827 0.2011597  5.640735 0.9980831
[10,] 100.2939 2.079470 0.009915805 10.03827 0.2011597  5.640735 0.9980809
[11,] 100.2939 4.158941 0.019831580 20.07655 0.4023193 11.281469 1.9961591
[12,] 100.2939 4.158941 0.019831563 20.07655 0.4023193 11.281469 1.9961579
[13,] 100.2939 4.158940 0.019831547 20.07655 0.4023193 11.281469 1.9961567
[14,] 100.2938 4.158940 0.019831530 20.07655 0.4023193 11.281468 1.9961555
[15,] 100.2938 4.158940 0.019831513 20.07655 0.4023193 11.281468 1.9961543
[16,] 100.2938 4.158940 0.019831497 20.07655 0.4023193 11.281468 1.9961531
[17,] 100.2938 4.158940 0.019831488 20.07655 0.4023193 11.281468 1.9961525
[18,] 100.2938 4.158940 0.019831485 20.07656 0.4023193 11.281467 1.9961523
[19,] 100.2937 4.158940 0.019831482 20.07656 0.4023193 11.281467 1.9961521
[20,] 100.2937 4.158940 0.019831479 20.07656 0.4023193 11.281467 1.9961519
[21,] 100.2937 4.158940 0.019831476 20.07656 0.4023193 11.281467 1.9961517
          arna      asuc      asli      dada      den     dgnuc     dnaa
 [1,] 1985.621  8.003186  8.003185 0.2004510 2.386351 0.1008502 10.03756
 [2,] 1985.621  8.003012  8.002051 0.2004511 2.402705 0.1008503 10.03756
 [3,] 1985.621  8.003027  8.003034 0.2004511 2.402830 0.1008504 10.03756
 [4,] 1985.622  8.003040  8.003040 0.2004512 2.402870 0.1008504 10.03756
 [5,] 1985.622  8.003050  8.003050 0.2004512 2.402897 0.1008504 10.03756
 [6,] 1985.622  8.003059  8.003059 0.2004512 2.402916 0.1008504 10.03756
 [7,] 1985.622  8.003068  8.003067 0.2004512 2.402935 0.1008504 10.03756
 [8,] 1985.622  8.003075  8.003075 0.2004512 2.402949 0.1008504 10.03756
 [9,] 1985.622  8.003082  8.003081 0.2004513 2.402959 0.1008504 10.03756
[10,] 1985.622  8.003088  8.003088 0.2004513 2.402969 0.1008504 10.03756
[11,] 3971.245 16.006189 16.006188 0.4009026 4.805953 0.2017008 20.07513
[12,] 3971.245 16.006202 16.006201 0.4009026 4.805962 0.2017008 20.07513
[13,] 3971.245 16.006214 16.006214 0.4009027 4.805971 0.2017008 20.07513
[14,] 3971.245 16.006227 16.006227 0.4009027 4.805980 0.2017008 20.07513
[15,] 3971.245 16.006240 16.006240 0.4009028 4.805990 0.2017008 20.07514
[16,] 3971.245 16.006253 16.006253 0.4009029 4.805999 0.2017008 20.07514
[17,] 3971.245 16.006262 16.006262 0.4009029 4.806003 0.2017008 20.07514
[18,] 3971.245 16.006269 16.006269 0.4009030 4.806005 0.2017008 20.07514
[19,] 3971.245 16.006277 16.006276 0.4009030 4.806007 0.2017008 20.07514
[20,] 3971.245 16.006284 16.006284 0.4009031 4.806009 0.2017009 20.07514
[21,] 3971.245 16.006291 16.006291 0.4009032 4.806011 0.2017009 20.07515
          dnag      gdna     gdrnr      gmpr     gmps     gnuc     gprt
 [1,]  6.826370  6.825859 0.1003440 0.5138721 1.595763 4.807078 3.738009
 [2,]  6.826370  6.825863 0.1003438 0.5138758 1.595763 4.807071 3.753990
 [3,]  6.826371  6.825864 0.1003439 0.5138767 1.595763 4.807084 3.753956
```

```
 [4,]  6.826371  6.825864 0.1003440 0.5138772 1.595763 4.807091 3.753883
 [5,]  6.826371  6.825865 0.1003440 0.5138774 1.595763 4.807094 3.753839
 [6,]  6.826371  6.825865 0.1003440 0.5138775 1.595763 4.807096 3.753808
 [7,]  6.826372  6.825865 0.1003440 0.5138776 1.595763 4.807098 3.753777
 [8,]  6.826372  6.825866 0.1003440 0.5138776 1.595762 4.807099 3.753754
 [9,]  6.826372  6.825866 0.1003440 0.5138777 1.595762 4.807099 3.753738
[10,]  6.826372  6.825866 0.1003440 0.5138777 1.595762 4.807100 3.753722
[11,] 13.652746 13.651733 0.2006880 1.0277553 3.191524 9.614200 7.507422
[12,] 13.652747 13.651734 0.2006879 1.0277553 3.191524 9.614200 7.507407
[13,] 13.652748 13.651735 0.2006879 1.0277552 3.191524 9.614201 7.507393
[14,] 13.652749 13.651736 0.2006879 1.0277551 3.191524 9.614201 7.507379
[15,] 13.652750 13.651737 0.2006878 1.0277551 3.191524 9.614201 7.507365
[16,] 13.652751 13.651738 0.2006878 1.0277550 3.191524 9.614201 7.507350
[17,] 13.652752 13.651739 0.2006877 1.0277550 3.191523 9.614201 7.507343
[18,] 13.652753 13.651740 0.2006877 1.0277549 3.191523 9.614201 7.507340
[19,] 13.652754 13.651741 0.2006877 1.0277548 3.191523 9.614201 7.507336
[20,] 13.652755 13.651742 0.2006876 1.0277547 3.191523 9.614201 7.507333
[21,] 13.652756 13.651743 0.2006876 1.0277547 3.191523 9.614201 7.507330
         grna      gua     hprt         hx      hxd     impd     inuc      mat
 [1,] 1323.532 1.154277 3.669760 0.04730928 1.191281 1.595762 2.642505 14.98849
 [2,] 1323.532 1.154508 3.684107 0.04732034 1.191442 1.595750 2.642393 14.98850
 [3,] 1323.532 1.154457 3.684108 0.04731749 1.191401 1.595750 2.642401 14.98850
 [4,] 1323.532 1.154419 3.684055 0.04731521 1.191368 1.595751 2.642408 14.98850
 [5,] 1323.533 1.154394 3.684017 0.04731365 1.191345 1.595752 2.642414 14.98850
 [6,] 1323.533 1.154377 3.683987 0.04731250 1.191328 1.595753 2.642419 14.98850
 [7,] 1323.533 1.154360 3.683956 0.04731134 1.191311 1.595753 2.642425 14.98850
 [8,] 1323.533 1.154347 3.683933 0.04731048 1.191298 1.595754 2.642429 14.98850
 [9,] 1323.533 1.154337 3.683914 0.04730985 1.191289 1.595754 2.642433 14.98850
[10,] 1323.533 1.154328 3.683896 0.04730923 1.191280 1.595755 2.642437 14.98850
[11,] 2647.066 2.308643 7.367766 0.09461768 2.382549 3.191511 5.284883 29.97699
[12,] 2647.066 2.308635 7.367749 0.09461730 2.382543 3.191512 5.284891 29.97699
[13,] 2647.066 2.308626 7.367731 0.09461691 2.382538 3.191513 5.284900 29.97699
[14,] 2647.066 2.308618 7.367713 0.09461652 2.382532 3.191514 5.284908 29.97699
[15,] 2647.066 2.308609 7.367696 0.09461614 2.382526 3.191515 5.284917 29.97699
[16,] 2647.066 2.308601 7.367678 0.09461575 2.382521 3.191516 5.284925 29.97699
[17,] 2647.066 2.308596 7.367669 0.09461565 2.382519 3.191517 5.284931 29.97699
[18,] 2647.066 2.308594 7.367666 0.09461572 2.382520 3.191517 5.284936 29.97699
[19,] 2647.066 2.308592 7.367663 0.09461579 2.382521 3.191518 5.284941 29.97699
[20,] 2647.066 2.308590 7.367660 0.09461586 2.382522 3.191518 5.284945 29.97699
[21,] 2647.066 2.308588 7.367656 0.09461593 2.382523 3.191519 5.284950 29.97699
       polyam    prpps      pyr     rnaa     rnag    trans       ua          x
 [1,] 1.007991 20.88492  9.99989 1985.551 1323.605 13.98050 2.314825 0.03071716
 [2,] 1.007991 20.88278 10.04333 1985.551 1323.605 13.98050 2.314828 0.03072109
 [3,] 1.007991 20.88275 10.04367 1985.551 1323.605 13.98050 2.314834 0.03072339
 [4,] 1.007991 20.88274 10.04378 1985.550 1323.605 13.98050 2.314842 0.03072430
 [5,] 1.007991 20.88274 10.04385 1985.550 1323.605 13.98050 2.314848 0.03072428
```

```
 [6,] 1.007991 20.88274 10.04390 1985.550 1323.605 13.98050 2.314854 0.03072385
 [7,] 1.007991 20.88273 10.04395 1985.550 1323.605 13.98050 2.314859 0.03072343
 [8,] 1.007991 20.88273 10.04399 1985.550 1323.605 13.98050 2.314863 0.03072290
 [9,] 1.007991 20.88273 10.04402 1985.550 1323.605 13.98050 2.314866 0.03072229
[10,] 1.007991 20.88273 10.04405 1985.550 1323.605 13.98050 2.314869 0.03072168
[11,] 2.015983 41.76546 20.08814 3971.101 2647.209 27.96101 4.629740 0.06144221
[12,] 2.015983 41.76546 20.08816 3971.101 2647.209 27.96101 4.629739 0.06144113
[13,] 2.015983 41.76546 20.08819 3971.101 2647.209 27.96101 4.629738 0.06144004
[14,] 2.015983 41.76546 20.08822 3971.101 2647.209 27.96101 4.629737 0.06143895
[15,] 2.015983 41.76545 20.08824 3971.101 2647.209 27.96101 4.629736 0.06143787
[16,] 2.015983 41.76545 20.08827 3971.101 2647.209 27.96101 4.629735 0.06143678
[17,] 2.015983 41.76545 20.08828 3971.101 2647.209 27.96101 4.629733 0.06143619
[18,] 2.015983 41.76545 20.08829 3971.101 2647.209 27.96101 4.629730 0.06143589
[19,] 2.015983 41.76545 20.08829 3971.101 2647.209 27.96101 4.629727 0.06143559
[20,] 2.015983 41.76545 20.08830 3971.101 2647.209 27.96101 4.629724 0.06143530
[21,] 2.015983 41.76545 20.08830 3971.101 2647.209 27.96101 4.629721 0.06143500
            xd R5P   Pi
 [1,] 2.314841  18 1400
 [2,] 2.314923  18 1400
 [3,] 2.314970  18 1400
 [4,] 2.314989  18 1400
 [5,] 2.314989  18 1400
 [6,] 2.314980  18 1400
 [7,] 2.314971  18 1400
 [8,] 2.314960  18 1400
 [9,] 2.314947  18 1400
[10,] 2.314935  18 1400
[11,] 4.629845  18 1400
[12,] 4.629823  18 1400
[13,] 4.629800  18 1400
[14,] 4.629778  18 1400
[15,] 4.629755  18 1400
[16,] 4.629733  18 1400
[17,] 4.629721  18 1400
[18,] 4.629714  18 1400
[19,] 4.629708  18 1400
[20,] 4.629702  18 1400
[21,] 4.629696  18 1400
attr(,"istate")
[1] 2
```

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

```
> simulate(curto, (-10):10, modulator = c(rep(1.1, 20), rep(0.9,
+     17)))
```

	time	PRPP	IMP	SAMP	ATP	SAM	Ade
[1,]	-10	5.000000	98.26340	0.198189000	2475.35000	3.991870	0.9847300000
[2,]	-9	5.017095	98.25819	0.198160810	2475.35236	3.991870	0.9849150437
[3,]	-8	5.017228	98.25854	0.198185483	2475.35358	3.991870	0.9848418902
[4,]	-7	5.017271	98.25887	0.198185683	2475.35413	3.991870	0.9848024315
[5,]	-6	5.017300	98.25916	0.198185950	2475.35431	3.991871	0.9847827859
[6,]	-5	5.017320	98.25940	0.198186169	2475.35433	3.991871	0.9847717607
[7,]	-4	5.017340	98.25965	0.198186387	2475.35434	3.991871	0.9847607355
[8,]	-3	5.017356	98.25986	0.198186571	2475.35432	3.991871	0.9847533693
[9,]	-2	5.017367	98.26005	0.198186727	2475.35425	3.991871	0.9847490095
[10,]	-1	5.017378	98.26024	0.198186883	2475.35419	3.991871	0.9847446496
[11,]	0	5.017125	98.26045	0.198186886	2475.28067	3.991870	0.9847033212
[12,]	1	4.942722	97.64947	0.176883677	2097.28379	3.896995	0.8013654770
[13,]	2	5.263423	96.43249	0.156422055	1747.75978	3.757725	0.6110696880
[14,]	3	5.678576	94.79475	0.136079226	1418.58072	3.604279	0.4333670466
[15,]	4	6.208070	92.84150	0.115204879	1106.95033	3.431260	0.2850609541
[16,]	5	6.906223	90.75119	0.093552797	813.79778	3.229711	0.1708134287
[17,]	6	7.882444	88.89621	0.071061866	543.48483	2.985441	0.0889335484
[18,]	7	9.371187	88.21632	0.048088202	305.51265	2.672575	0.0360469255
[19,]	8	11.953795	91.81694	0.025764928	120.35685	2.240272	0.0088253275
[20,]	9	16.535834	113.06819	0.010326410	28.61333	1.668489	0.0009198177
[21,]	10	19.417960	167.89378	0.007564643	14.10909	1.380957	0.0003500507

	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	9.5198359	5.059734
[3,]	24.79298	410.2235	6.014136	3.025813	28680.49	5179.340	9.5193252	5.059924
[4,]	24.79296	410.2242	6.014137	3.025814	28680.49	5179.341	9.5189149	5.059998
[5,]	24.79295	410.2245	6.014137	3.025814	28680.49	5179.341	9.5186350	5.059997
[6,]	24.79295	410.2247	6.014138	3.025814	28680.49	5179.341	9.5184272	5.059962
[7,]	24.79294	410.2248	6.014138	3.025814	28680.49	5179.341	9.5182194	5.059927
[8,]	24.79293	410.2249	6.014139	3.025814	28680.49	5179.341	9.5180642	5.059883
[9,]	24.79292	410.2250	6.014139	3.025814	28680.49	5179.342	9.5179524	5.059833
[10,]	24.79291	410.2251	6.014139	3.025814	28680.49	5179.342	9.5178405	5.059783
[11,]	24.79285	410.2251	6.014140	3.025814	28680.56	5179.342	9.5178181	5.059732
[12,]	24.49245	421.2855	6.012597	3.026378	29048.35	5179.342	9.8444359	5.089213
[13,]	24.22826	449.4133	6.007924	3.029316	29371.97	5179.341	9.6202672	5.150227
[14,]	24.00077	489.7226	5.999331	3.035443	29664.28	5179.341	8.8684786	5.210686
[15,]	23.81307	540.3163	5.985946	3.045135	29929.99	5179.342	7.6660475	5.253933
[16,]	23.67127	601.3511	5.966937	3.058756	30168.10	5179.346	6.1109339	5.268473
[17,]	23.58604	674.7773	5.941311	3.076830	30372.60	5179.352	4.3427577	5.243750
[18,]	23.57661	765.1320	5.907549	3.100216	30530.06	5179.361	2.5829892	5.171288
[19,]	23.68099	882.3571	5.862859	3.130456	30611.65	5179.371	1.1873211	5.052278
[20,]	23.97285	1045.5427	5.802604	3.170452	30562.35	5179.380	0.5830086	4.921096
[21,]	24.46767	1241.2562	5.730521	3.222263	30416.42	5179.387	0.9064364	4.893043

	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 2.07946892 0.0099167491 10.03827 0.2011596 5.64073249
 [3,]  5.508098 100.2932 2.07946992 0.0099163440 10.03827 0.2011597 5.64073423
 [4,]  5.507735 100.2933 2.07947037 0.0099161254 10.03827 0.2011597 5.64073496
 [5,]  5.507502 100.2935 2.07947051 0.0099160166 10.03827 0.2011597 5.64073515
 [6,]  5.507337 100.2936 2.07947052 0.0099159556 10.03827 0.2011597 5.64073511
 [7,]  5.507171 100.2937 2.07947054 0.0099158945 10.03827 0.2011597 5.64073508
 [8,]  5.507048 100.2937 2.07947052 0.0099158537 10.03827 0.2011597 5.64073499
 [9,]  5.506960 100.2938 2.07947046 0.0099158296 10.03827 0.2011597 5.64073485
[10,]  5.506871 100.2939 2.07947041 0.0099158054 10.03827 0.2011597 5.64073471
[11,]  5.506830 100.2939 2.28735155 0.0109071342 11.04210 0.2212750 6.20466072
[12,]  5.892429 100.2962 1.94771176 0.0097386673 11.04159 0.2176905 5.42997225
[13,]  6.367382 100.3093 1.63201630 0.0083896258 11.04152 0.2139882 4.68398141
[14,]  7.064006 100.3354 1.33295544 0.0069448588 11.04224 0.2100279 3.95361052
[15,]  8.050277 100.3720 1.04790398 0.0055157991 11.04350 0.2055890 3.23245294
[16,]  9.340340 100.4133 0.77753189 0.0041617864 11.04501 0.2003269 2.51911795
[17,] 10.921571 100.4519 0.52559231 0.0029065565 11.04652 0.1936392 1.81754123
[18,] 12.746876 100.4782 0.30060453 0.0017687653 11.04769 0.1843236 1.14214281
[19,] 14.684629 100.4821 0.12177942 0.0008157266 11.04784 0.1697391 0.53977961
[20,] 16.448516 100.4569 0.03022655 0.0002351953 11.04619 0.1491195 0.17017024
[21,] 18.788481 100.4120 0.01522409 0.0001382499 11.04728 0.1414428 0.09615958
          aprt     arna      asuc      asli      dada       den     dgnuc
 [1,] 0.9963412 1985.621  8.003186  8.003185 0.2004510   2.386351 0.1008502
 [2,] 0.9981829 1985.621  8.003012  8.002051 0.2004511   2.402705 0.1008503
 [3,] 0.9981402 1985.621  8.003027  8.003034 0.2004511   2.402830 0.1008504
 [4,] 0.9981143 1985.622  8.003040  8.003040 0.2004512   2.402870 0.1008504
 [5,] 0.9981021 1985.622  8.003050  8.003050 0.2004512   2.402897 0.1008504
 [6,] 0.9980957 1985.622  8.003059  8.003059 0.2004512   2.402916 0.1008504
 [7,] 0.9980894 1985.622  8.003068  8.003067 0.2004512   2.402935 0.1008504
 [8,] 0.9980853 1985.622  8.003075  8.003075 0.2004512   2.402949 0.1008504
 [9,] 0.9980831 1985.622  8.003082  8.003081 0.2004513   2.402959 0.1008504
[10,] 0.9980809 1985.622  8.003088  8.003088 0.2004513   2.402969 0.1008504
[11,] 1.0978528 2184.181  8.803467  8.803645 0.2204964   2.643019 0.1109354
[12,] 1.0660253 2173.664  9.186566  9.207424 0.2204398   2.660519 0.1109561
[13,] 1.0386136 2172.114  9.673655  9.693909 0.2202685   3.119445 0.1110638
[14,] 0.9851800 2173.706 10.276056 10.296607 0.2199535   3.764108 0.1112885
[15,] 0.9175216 2174.529 11.030708 11.051877 0.2194627   4.699274 0.1116438
[16,] 0.8430160 2171.336 12.022928 12.046396 0.2187658   6.156007 0.1121432
[17,] 0.7624598 2160.055 13.443368 13.464610 0.2178263   8.679679 0.1128058
[18,] 0.6695181 2133.299 15.780745 15.810369 0.2165885  13.822781 0.1136632
[19,] 0.5545128 2074.302 20.632539 20.652515 0.2149500  27.525386 0.1147719
[20,] 0.3775477 1973.592 32.748830 32.701788 0.2127409  72.008716 0.1162383
[21,] 0.3490101 1948.011 47.040728 47.041162 0.2100981 111.815452 0.1181378
         dnaa     dnag     gdna     gdrnr      gmpr      gmps      gnuc
 [1,] 10.03756 6.826370 6.825859 0.1003440 0.5138721 1.5957628  4.807078
 [2,] 10.03756 6.826370 6.825863 0.1003438 0.5138758 1.5957629  4.807071
 [3,] 10.03756 6.826371 6.825864 0.1003439 0.5138767 1.5957629  4.807084
```

```
 [4,] 10.03756 6.826371 6.825864 0.1003440 0.5138772 1.5957628  4.807091
 [5,] 10.03756 6.826371 6.825865 0.1003440 0.5138774 1.5957627  4.807094
 [6,] 10.03756 6.826371 6.825865 0.1003440 0.5138775 1.5957626  4.807096
 [7,] 10.03756 6.826372 6.825865 0.1003440 0.5138776 1.5957625  4.807098
 [8,] 10.03756 6.826372 6.825866 0.1003440 0.5138776 1.5957624  4.807099
 [9,] 10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957624  4.807099
[10,] 10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957623  4.807100
[11,] 11.04132 7.509010 7.508453 0.1103784 0.5652676 1.7553315  5.287810
[12,] 11.04132 7.509010 7.508105 0.1115855 0.5885858 1.7174180  5.415951
[13,] 11.04132 7.509009 7.508057 0.1145715 0.6300822 1.6773409  5.740334
[14,] 11.04132 7.509008 7.508551 0.1186866 0.6856204 1.6333923  6.201703
[15,] 11.04132 7.509010 7.509406 0.1236247 0.7541553 1.5834991  6.775465
[16,] 11.04133 7.509016 7.510434 0.1293001 0.8371523 1.5246474  7.460556
[17,] 11.04134 7.509025 7.511460 0.1357866 0.9389361 1.4517080  8.275615
[18,] 11.04136 7.509038 7.512251 0.1433424 1.0690116 1.3546668  9.266561
[19,] 11.04138 7.509052 7.512355 0.1525637 1.2490303 1.2122507 10.535031
[20,] 11.04140 7.509064 7.511234 0.1644992 1.4935805 1.0222929 12.273360
[21,] 11.04142 7.509075 7.511978 0.1777218 1.6420621 0.9422078 14.322906
          gprt     grna      gua     hprt          hx       hxd     impd
 [1,] 3.738009 1323.532 1.154277 3.669760 0.047309283 1.1912809 1.595762
 [2,] 3.753990 1323.532 1.154508 3.684107 0.047320338 1.1914425 1.595750
 [3,] 3.753956 1323.532 1.154457 3.684108 0.047317495 1.1914009 1.595750
 [4,] 3.753883 1323.532 1.154419 3.684055 0.047315211 1.1913676 1.595751
 [5,] 3.753839 1323.533 1.154394 3.684017 0.047313653 1.1913448 1.595752
 [6,] 3.753808 1323.533 1.154377 3.683987 0.047312496 1.1913279 1.595753
 [7,] 3.753777 1323.533 1.154360 3.683956 0.047311339 1.1913110 1.595753
 [8,] 3.753754 1323.533 1.154347 3.683933 0.047310475 1.1912984 1.595754
 [9,] 3.753738 1323.533 1.154337 3.683914 0.047309852 1.1912893 1.595754
[10,] 3.753722 1323.533 1.154328 3.683896 0.047309230 1.1912802 1.595755
[11,] 4.128831 1191.178 1.038891 3.315313 0.042578194 1.0721505 1.436180
[12,] 4.041294 1185.442 1.074649 3.332970 0.044217999 1.0959241 1.435266
[13,] 4.166195 1184.597 1.117120 3.571983 0.043091831 1.0796378 1.431190
[14,] 4.300092 1185.465 1.176643 3.791719 0.039338371 1.0240198 1.425053
[15,] 4.493037 1185.914 1.256102 3.972824 0.033415306 0.9314894 1.417427
[16,] 4.779875 1184.172 1.353009 4.088378 0.025921841 0.8038525 1.408822
[17,] 5.209661 1178.020 1.463059 4.087819 0.017681651 0.6438046 1.400074
[18,] 5.883946 1163.428 1.580597 3.879695 0.009881040 0.4592891 1.393250
[19,] 7.047667 1131.253 1.696488 3.369698 0.004137535 0.2771250 1.395100
[20,] 8.900278 1076.330 1.795489 2.843564 0.001865440 0.1745401 1.430468
[21,] 9.289114 1062.379 1.918957 2.949907 0.003058040 0.2325282 1.507295
          inuc       mat    polyam     prpps       pyr     rnaa     rnag
 [1,] 2.642505 14.988492 1.0079912  20.88492  9.999890 1985.551 1323.605
 [2,] 2.642393 14.988495 1.0079911  20.88278 10.043331 1985.551 1323.605
 [3,] 2.642401 14.988496 1.0079913  20.88275 10.043669 1985.551 1323.605
 [4,] 2.642408 14.988496 1.0079913  20.88274 10.043779 1985.550 1323.605
 [5,] 2.642414 14.988496 1.0079913  20.88274 10.043851 1985.550 1323.605
```

```
 [6,] 2.642419 14.988496 1.0079913  20.88274 10.043903 1985.550 1323.605
 [7,] 2.642425 14.988496 1.0079913  20.88273 10.043954 1985.550 1323.605
 [8,] 2.642429 14.988496 1.0079913  20.88273 10.043993 1985.550 1323.605
 [9,] 2.642433 14.988496 1.0079913  20.88273 10.044021 1985.550 1323.605
[10,] 2.642437 14.988496 1.0079913  20.88273 10.044049 1985.550 1323.605
[11,] 2.378198 13.489566 0.9071922  18.79474  9.039065 1787.000 1191.247
[12,] 2.366360 13.239528 0.8877636  20.23737  8.869168 1809.915 1206.523
[13,] 2.342738 13.047290 0.8591579  21.86961  9.606308 1830.079 1219.965
[14,] 2.310853 12.830948 0.8275172  23.88594 10.578642 1848.293 1232.106
[15,] 2.272682 12.575707 0.7916783  26.53075 11.846790 1864.848 1243.142
[16,] 2.231654 12.262643 0.7497004  30.24315 13.563801 1879.684 1253.032
[17,] 2.195086 11.857998 0.6984706  35.95847 16.043724 1892.426 1261.526
[18,] 2.181645 11.293455 0.6322334  46.12489 19.985957 1902.236 1268.066
[19,] 2.252596 10.420598 0.5394004  69.23711 27.225646 1907.320 1271.455
[20,] 2.660831  9.330366 0.4137438 129.99287 41.109951 1904.248 1269.407
[21,] 3.650671  9.073414 0.3489816 176.61461 50.415536 1895.156 1263.346
          trans       ua          x       xd R5P   Pi
 [1,] 13.980504 2.314825 0.03071716 2.314841  18 1400
 [2,] 13.980503 2.314828 0.03072109 2.314923  18 1400
 [3,] 13.980504 2.314834 0.03072339 2.314970  18 1400
 [4,] 13.980504 2.314842 0.03072430 2.314989  18 1400
 [5,] 13.980504 2.314848 0.03072428 2.314989  18 1400
 [6,] 13.980504 2.314854 0.03072385 2.314980  18 1400
 [7,] 13.980504 2.314859 0.03072343 2.314971  18 1400
 [8,] 13.980504 2.314863 0.03072290 2.314960  18 1400
 [9,] 13.980504 2.314866 0.03072229 2.314947  18 1400
[10,] 13.980504 2.314869 0.03072168 2.314935  18 1400
[11,] 12.582454 2.083385 0.02764896 2.083430  18 1400
[12,] 12.482971 2.083492 0.02797209 2.090098  18 1400
[13,] 12.333955 2.084089 0.02864682 2.103842  18 1400
[14,] 12.165422 2.085290 0.02932335 2.117390  18 1400
[15,] 11.969522 2.086970 0.02981212 2.127038  18 1400
[16,] 11.732785 2.088872 0.02997735 2.130273  18 1400
[17,] 11.432203 2.090645 0.02969667 2.124769  18 1400
[18,] 11.022091 2.091855 0.02888160 2.108570  18 1400
[19,] 10.398636 2.092033 0.02756756 2.081741  18 1400
[20,]  9.435041 2.090872 0.02615456 2.051836  18 1400
[21,]  8.864139 2.088808 0.02585722 2.045395  18 1400
attr(,"istate")
[1] 2
```

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 = simulate(morr, seq(-20, 0, 1))
```

```
> morr$species$EMTX$ic = 1
> out2 = simulate(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, 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

$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



$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: 0x1830998>
```

```
$reactions$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: 0xd33e08>


$reactions$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: 0x947cb8>


$reactions$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: 0x8d6818>


$reactions$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: 0x1551ca0>


$reactions$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: 0x7fd330>


$reactions$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: 0x1a34ec8>


$reactions$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
}
<environment: 0x790d20>


$reactions$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: 0x893c30>


$reactions$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: 0x16143c8>


$reactions$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
}
<environment: 0x1853c58>


$reactions$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: 0xb73f28>


$reactions$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: 0x17e1418>


$reactions$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: 0x188a758>


$reactions$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: 0x837e68>


$reactions$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: 0x225db60>


$reactions$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
}
<environment: 0xe040f8>


$reactions$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: 0x2224238>


$reactions$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: 0xebe0a8>


$reactions$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: 0xf784c0>


$reactions$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: 0x115ac90>


$reactions$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: 0x1163160>


$reactions$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: 0x93ebe0>


$reactions$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: 0x18bdbe8>


$reactions$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: 0x2233048>


$reactions$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: 0x181af18>


$reactions$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: 0xbd4888>


$reactions$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: 0x93a540>


$reactions$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: 0x187bad0>


$reactions$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 * PRPPˆfprpps1 * ATPˆfprpps4 * GTPˆfprpps8 * R5Pˆfprpps17 *
    Piˆfprpps18

$reactions$prpps$strLaw
[1] "aprpps*PRPPˆfprpps1*ATPˆfprpps4*GTPˆfprpps8*R5Pˆfprpps17*Piˆfprpps18"

$reactions$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 * PRPPˆfprpps1 * ATPˆfprpps4 * GTPˆfprpps8 * R5Pˆfprpps17 *
        Piˆfprpps18
}
<environment: 0x1663b40>


$reactions$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: 0x10cff88>


$reactions$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: 0x16f4bf0>


$reactions$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: 0x982bc0>


$reactions$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: 0x1783878>


$reactions$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: 0x222a4c8>


$reactions$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: 0x21c9020>


$reactions$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: 0x8e5c38>



$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] "SBML"
```