

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 ^f fada4	2.079466999
ade	2	aade*Ade ^f fade6	0.009915724
adna	3	aadna*dATP ^f fdnap9*dGTP ^f fdnap10	10.038261346
adrnr	4	aadrnr*ATP ^f fadrnr4*dATP ^f fadrnr9*dGTP ^f fadrnr10	0.201159500
ampd	5	aampd*ATP ^f fampd4*GTP ^f fampd8*Pi ^f fampd18	5.640727920
aprt	6	aaprt*PRPP ^f faprt1*ATP ^f faprt4*Ade ^f 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 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
> 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	gmpr	gnuc	gprr
[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

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[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

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[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

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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"	"gprr"	"grna"	"gua"	"hprr"	"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"
 gprrt
 "agprrt*PRPP^fgprrt1*GTP^fgprrt8*Gua^fgprrt15"
 grna
 "agrna*ATP^frnap4*GTP^frnap8"
 gua
 "agua*Gua^fgua15"
 hprrt
 "ahprrt*PRPP^fhprrt1*IMP^fhprrt2*HX^fhprrt13"
 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      adnr      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    0
IMP     0    0    1    0    0    0    0    0    1    0    0    0   -1
SAMP    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
SAM     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
XMP     0    0    0   -1    0    0    0    0    0    0    0    0    1
GTP     0   -1   -1    1   -1    1   -1    0    0    0    0    0    0

```

dATP	0	0	0	0	0	0	0	0	0	0	0	0
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	0
IMP	-1	0	0	0	0	0	0	0	0	0	0	0
SAMP	0	0	0	0	0	0	0	0	0	0	0	0
ATP	0	-1	0	0	0	1	0	1	0	0	0	0
SAM	0	1	-1	0	0	0	0	-1	0	0	0	0
Ade	0	0	1	0	0	0	0	0	0	0	0	0
XMP	0	0	0	0	0	0	0	0	0	0	0	0
GTP	0	0	0	0	0	0	1	0	0	0	0	0
dATP	0	0	0	0	0	0	0	0	0	0	0	0
dGTP	0	0	0	0	0	0	0	0	0	0	0	0
RNA	0	0	0	0	0	-1	-1	0	0	0	0	0
DNA	0	0	0	0	0	0	0	0	0	0	0	0
HX	1	0	0	0	0	0	0	0	0	0	0	0
Xa	0	0	0	0	0	0	0	0	0	-1	-1	0
Gua	0	0	0	0	0	0	0	0	0	0	0	0
UA	0	0	0	0	0	0	0	0	-1	0	1	0

\$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
gmpr	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
gprrt     3.738009e+00
grna      1.323532e+03
gua        1.154277e+00
hprrt     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. $2.4 \cdot 60 = 144$ 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
$reactions$aada
$reactions$aada$id
[1] "ada"

$reactions$aada$reversible
[1] FALSE

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

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

$reactions$aada$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: 0xf0af78>

```

```

$reactions$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: 0x1a8b0e0>

$reactions$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: 0x17b8de8>

```

```

$reactions$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
  adrnr  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: 0x15414b8>

```

```

$reactions$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"

```

```

$reactions$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>
<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: 0x19b2238>

```

```

$reactions$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: 0x1b46c70>

$reactions$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
```

```
$reactions$aarna$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: 0xf8c018>
```

```
$reactions$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>
    <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: 0x1546b00>

$reactions$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: 0x162af10>

$reactions$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: 0x101fb48>

$reactions$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: 0x184da30>

```

```

$reactions$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: 0x1527070>

$reactions$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: 0x21fefe0>
```

```
$reactions$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: 0x15f5590>
```

```
$reactions$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: 0xb9a320>

$reactions$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: 0x18a48e0>

$reactions$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: 0xe927d0>

```

```

$reactions$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: 0x1729fc8>

$reactions$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: 0x825df8>

$reactions$gpert
$reactions$gpert$id
[1] "gpert"

$reactions$gpert$reversible
[1] FALSE

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

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

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

```

```
$reactions$gpert$parameters
  agprt fgprt1 fgprt8 fgprt15
361.69   1.20  -1.20   0.42
```

```
$reactions$gpert$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>
```

```
$reactions$gpert$exprLaw
```

```
agprt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15
```

```
$reactions$gpert$strLaw
```

```
[1] "agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15"
```

```
$reactions$gpert$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"]
    agrpt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15
  }
<environment: 0xa62158>

```

```

$reactions$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: 0x19d5598>

$reactions$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: 0x21e8678>

$reactions$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>

```

```

$reactions$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: 0x1a9b360>

```

```

$reactions$hX
$reactions$hX$id
[1] "hX"

```

```

$reactions$hX$reversible
[1] FALSE

```

```

$reactions$hreactants
[1] "HX"

$reactions$hparameters
      ahx      fhx13
0.003793 1.120000

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

$reactions$hexprLaw
ahx * HX^fhx13

$reactions$hstrLaw
[1] "ahx*HX^fhx13"

$reactions$hlaw
function (r, p = NULL)
{
  ahx = p["ahx"]
  fhx13 = p["fhx13"]
  HX = r["HX"]
  ahx * HX^fhx13
}
<environment: 0x1821120>

$reactions$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: 0x10d99d8>

$reactions$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: 0x2109b38>

```

```

$reactions$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: 0x8f9be8>

$reactions$mat
$reactions$mat$nid
[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: 0x1006ab0>

$reactions$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: 0x84fc70>

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

$reactions$prpps$reversible
[1] FALSE

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

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

```

```
$reactions$prpps$products
```

```
[1] "PRPP"
```

```
$reactions$prpps$parameters
```

```
aprpps fprpps1 fprpps4 fprpps8 fprpps17 fprpps18  
0.90 -0.03 -0.45 -0.04 0.65 0.70
```

```
$reactions$prpps$mathmlLaw
```

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

```

    <ci>fprpps18</ci>
  </apply>
</apply>

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

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

$reactions$prpps$law
function (r, p = NULL)
{
  aprpps = p["aprpps"]
  fprpps1 = p["fprpps1"]
  fprpps4 = p["fprpps4"]
  fprpps8 = p["fprpps8"]
  fprpps17 = p["fprpps17"]
  fprpps18 = p["fprpps18"]
  R5P = r["R5P"]
  ATP = r["ATP"]
  GTP = r["GTP"]
  Pi = r["Pi"]
  PRPP = r["PRPP"]
  aprpps * PRPP^fprpps1 * ATP^fprpps4 * GTP^fprpps8 * R5P^fprpps17 *
    Pi^fprpps18
}
<environment: 0x9f19f8>

$reactions$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: 0x100bdc0>

$reactions$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 frnan1
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: 0x190aba8>

$reactions$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: 0x2190ea8>

$reactions$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: 0xbbc8b8>

$reactions$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
ua * UA^fua16

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

$reactions$ua$law
function (r, p = NULL)
{
  ua = p["ua"]
  fua16 = p["fua16"]
  UA = r["UA"]
  ua * UA^fua16
}
<environment: 0x1928dc0>

```

```

$reactions$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: 0x2101f70>

$reactions$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: 0x87e078>

```

```
$htmlNotes
```

```

<notes>
<body xmlns="http://www.w3.org/1999/xhtml">
  <p>This is a purine metabolism model that is geared toward studies of gout.</p>
  <p>The model is fully described in Curto et al., MBSC 151 (1998) pp 1-49</p>
  <p>The model uses Generalized Mass Action (GMA;i.e. power law) descriptions of reaction ra
  <p>Such descriptions are local approximations that assume independent substrate binding.</p>
  <p/>
  <p>The de novo purine flux vden= 2.39 is in umole/min/KG, i.e. 2.4*60=144 uM/h if we let e
  <p>liter of water. Morrison and Allegra (JBC, 1989) have vden at 650 uM/h (model) and 415
  <p>The IC&apos;s below have been set to the system&apos;s steady state.</p>
  <p>The units in this model are micromolar(uM) and minutes.</p>
  <p>A cell volume of 1 is used so that amounts and concentrations are the same thing.</p>
</body>
</notes>

```

```

attr("class")
[1] "SBML"

```