Quick Intro to SBMLR

Tom Radivoyevitch

October 14, 2013

Introduction

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

Model import, export, editing and viewing

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

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

```
      index                                          Laws initialFluxes
ada       1                                aada*ATP^fada4   2.079466999
ade       2                                aade*Ade^fade6   0.009915724
adna      3               aadna*dATP^fdnap9*dGTP^fdnap10  10.038261346
adrnr     4 aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10   0.201159500
ampd      5        aampd*ATP^fampd4*GTP^fampd8*Pi^fampd18   5.640727920
aprt      6       aaprt*PRPP^faprt1*ATP^faprt4*Ade^faprt6   0.998075329
```

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

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

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

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

```
     index initialConcentrations boundaryConditions
PRPP  TRUE                  TRUE               TRUE
IMP   TRUE                  TRUE               TRUE
SAMP  TRUE                  TRUE               TRUE
ATP   TRUE                  TRUE               TRUE
SAM   TRUE                  TRUE               TRUE
Ade   TRUE                  TRUE               TRUE
```

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

```
      index Laws initialFluxes
ada    TRUE TRUE          TRUE
ade    TRUE TRUE          TRUE
adna   TRUE TRUE          TRUE
adrnr  TRUE TRUE          TRUE
ampd   TRUE TRUE          TRUE
aprt   TRUE TRUE          TRUE
```

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

Model simulation

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

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

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

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

	time	PRPP	IMP	SAMP	ATP	SAM	Ade	XMP
1	-10	5.000000	98.26340	0.1981890	2475.350	3.991870	0.9847300	24.79300
2	-9	5.017097	98.25819	0.1981848	2475.352	3.991870	0.9849151	24.79299
3	-8	5.017231	98.25855	0.1981853	2475.354	3.991870	0.9848325	24.79298
4	-7	5.017280	98.25890	0.1981857	2475.354	3.991871	0.9847894	24.79296
5	-6	5.017315	98.25922	0.1981860	2475.355	3.991871	0.9847674	24.79295
6	-5	5.017341	98.25951	0.1981863	2475.355	3.991871	0.9847554	24.79294
7	-4	5.017360	98.25977	0.1981865	2475.354	3.991871	0.9847480	24.79293
8	-3	5.017375	98.26000	0.1981867	2475.354	3.991871	0.9847433	24.79293
9	-2	5.017386	98.26020	0.1981869	2475.354	3.991871	0.9847401	24.79292
10	-1	5.017395	98.26039	0.1981870	2475.354	3.991870	0.9847379	24.79291
11	0	5.017402	98.26058	0.1981872	2475.354	3.991870	0.9847361	24.79290
12	1	5.017411	98.26086	0.1981874	2475.354	3.991870	0.9847342	24.79289
13	2	5.017415	98.26110	0.1981876	2475.354	3.991870	0.9847331	24.79288
14	3	5.017419	98.26131	0.1981877	2475.354	3.991870	0.9847324	24.79287
15	4	5.017421	98.26150	0.1981879	2475.354	3.991870	0.9847319	24.79286
16	5	5.017422	98.26167	0.1981880	2475.354	3.991870	0.9847317	24.79286
17	6	5.017422	98.26181	0.1981881	2475.353	3.991870	0.9847316	24.79285
18	7	5.017422	98.26194	0.1981882	2475.353	3.991870	0.9847315	24.79285
19	8	5.017422	98.26206	0.1981883	2475.353	3.991870	0.9847315	24.79284
20	9	5.017422	98.26216	0.1981884	2475.353	3.991870	0.9847315	24.79284
21	10	5.017422	98.26226	0.1981885	2475.353	3.991870	0.9847315	24.79284

	GTP	dATP	dGTP	RNA	DNA	HX	Xa	Gua
1	410.2230	6.014130	3.025810	28680.50	5179.340	9.517850	5.059410	5.506380
2	410.2223	6.014135	3.025813	28680.50	5179.340	9.519836	5.059734	5.508591
3	410.2237	6.014136	3.025813	28680.49	5179.340	9.519291	5.059957	5.508056
4	410.2244	6.014137	3.025814	28680.49	5179.341	9.518845	5.060051	5.507660
5	410.2248	6.014137	3.025814	28680.49	5179.341	9.518494	5.060063	5.507373
6	410.2250	6.014138	3.025814	28680.49	5179.341	9.518221	5.060026	5.507162
7	410.2251	6.014138	3.025814	28680.49	5179.341	9.518010	5.059964	5.507004
8	410.2251	6.014139	3.025814	28680.49	5179.341	9.517849	5.059891	5.506887
9	410.2251	6.014139	3.025814	28680.49	5179.342	9.517728	5.059816	5.506798
10	410.2251	6.014139	3.025814	28680.49	5179.342	9.517638	5.059744	5.506731
11	410.2251	6.014140	3.025814	28680.49	5179.342	9.517565	5.059668	5.506674
12	410.2251	6.014141	3.025814	28680.49	5179.342	9.517495	5.059567	5.506611
13	410.2251	6.014142	3.025814	28680.49	5179.343	9.517470	5.059494	5.506575
14	410.2251	6.014142	3.025815	28680.49	5179.343	9.517462	5.059439	5.506549
15	410.2251	6.014143	3.025815	28680.49	5179.344	9.517471	5.059403	5.506534
16	410.2251	6.014144	3.025815	28680.49	5179.344	9.517490	5.059382	5.506526
17	410.2251	6.014145	3.025815	28680.49	5179.344	9.517515	5.059373	5.506522
18	410.2251	6.014146	3.025815	28680.49	5179.345	9.517541	5.059370	5.506520
19	410.2251	6.014147	3.025815	28680.49	5179.345	9.517566	5.059371	5.506519
20	410.2251	6.014148	3.025815	28680.49	5179.346	9.517590	5.059375	5.506519
21	410.2251	6.014148	3.025816	28680.49	5179.346	9.517612	5.059380	5.506518

	UA	ada	ade	adna	adrnr	ampd	aprt
1	100.2930	2.079467	0.009915724	10.03826	0.2011595	5.640728	0.9963412

2	100.2931	2.079469	0.009916749	10.03827	0.2011596	5.640732	0.9981831	
3	100.2932	2.079470	0.009916292	10.03827	0.2011597	5.640735	0.9981332	
4	100.2933	2.079471	0.009916053	10.03827	0.2011597	5.640735	0.9981052	
5	100.2935	2.079471	0.009915932	10.03827	0.2011597	5.640736	0.9980919	
6	100.2936	2.079471	0.009915865	10.03827	0.2011597	5.640735	0.9980853	
7	100.2938	2.079471	0.009915824	10.03827	0.2011597	5.640735	0.9980816	
8	100.2939	2.079471	0.009915798	10.03827	0.2011597	5.640735	0.9980795	
9	100.2940	2.079470	0.009915780	10.03827	0.2011597	5.640735	0.9980783	
10	100.2940	2.079470	0.009915768	10.03827	0.2011597	5.640735	0.9980775	
11	100.2941	4.158941	0.019831516	20.07655	0.4023194	11.281469	1.9961538	
12	100.2941	4.158940	0.019831495	20.07655	0.4023193	11.281468	1.9961526	
13	100.2940	4.158940	0.019831483	20.07655	0.4023193	11.281468	1.9961521	
14	100.2940	4.158940	0.019831475	20.07655	0.4023193	11.281467	1.9961516	
15	100.2939	4.158940	0.019831470	20.07655	0.4023193	11.281467	1.9961514	
16	100.2939	4.158940	0.019831467	20.07655	0.4023193	11.281467	1.9961513	
17	100.2938	4.158940	0.019831466	20.07655	0.4023193	11.281467	1.9961512	
18	100.2937	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
19	100.2937	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
20	100.2936	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
21	100.2936	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	

	arna	asuc	asli	dada	den	dgnuc	dnaa	dnag
1	1985.621	8.003186	8.003185	0.2004510	2.386351	0.1008502	10.03756	6.826370
2	1985.621	8.003012	8.003012	0.2004511	2.402707	0.1008503	10.03756	6.826370
3	1985.621	8.003028	8.003027	0.2004512	2.402833	0.1008504	10.03756	6.826371
4	1985.622	8.003042	8.003041	0.2004512	2.402879	0.1008504	10.03756	6.826371
5	1985.622	8.003053	8.003053	0.2004512	2.402911	0.1008504	10.03756	6.826371
6	1985.622	8.003064	8.003063	0.2004512	2.402935	0.1008504	10.03756	6.826371
7	1985.622	8.003072	8.003072	0.2004512	2.402953	0.1008504	10.03756	6.826372
8	1985.622	8.003080	8.003080	0.2004512	2.402967	0.1008504	10.03756	6.826372
9	1985.622	8.003087	8.003087	0.2004513	2.402977	0.1008504	10.03756	6.826372
10	1985.622	8.003093	8.003093	0.2004513	2.402985	0.1008504	10.03756	6.826372
11	3971.245	16.006199	16.006199	0.4009026	4.805985	0.2017008	20.07513	13.652746
12	3971.245	16.006217	16.006217	0.4009026	4.806000	0.2017008	20.07513	13.652747
13	3971.245	16.006233	16.006233	0.4009027	4.806008	0.2017008	20.07513	13.652748
14	3971.245	16.006247	16.006247	0.4009027	4.806014	0.2017008	20.07513	13.652749
15	3971.245	16.006260	16.006259	0.4009028	4.806017	0.2017008	20.07514	13.652750
16	3971.245	16.006270	16.006270	0.4009028	4.806018	0.2017008	20.07514	13.652751
17	3971.245	16.006280	16.006280	0.4009029	4.806019	0.2017008	20.07514	13.652752
18	3971.245	16.006288	16.006288	0.4009030	4.806018	0.2017008	20.07514	13.652753
19	3971.245	16.006296	16.006296	0.4009030	4.806018	0.2017008	20.07514	13.652754
20	3971.245	16.006303	16.006303	0.4009031	4.806018	0.2017009	20.07514	13.652755
21	3971.245	16.006309	16.006309	0.4009031	4.806017	0.2017009	20.07515	13.652756

	gdna	gdrnr	gmpr	gmps	gnuc	gprt	grna	gua
1	6.825859	0.1003440	0.5138721	1.595763	4.807078	3.738009	1323.532	1.154277
2	6.825863	0.1003438	0.5138758	1.595763	4.807071	3.753992	1323.532	1.154508
3	6.825864	0.1003439	0.5138768	1.595763	4.807085	3.753944	1323.532	1.154452

4	6.825864	0.1003440	0.5138774	1.595763	4.807093	3.753867	1323.533	1.154411
5	6.825865	0.1003440	0.5138776	1.595763	4.807097	3.753812	1323.533	1.154381
6	6.825865	0.1003440	0.5138777	1.595763	4.807099	3.753773	1323.533	1.154359
7	6.825865	0.1003440	0.5138778	1.595762	4.807100	3.753744	1323.533	1.154342
8	6.825866	0.1003440	0.5138777	1.595762	4.807100	3.753723	1323.533	1.154330
9	6.825866	0.1003440	0.5138777	1.595762	4.807101	3.753708	1323.533	1.154320
10	6.825866	0.1003440	0.5138777	1.595762	4.807101	3.753696	1323.533	1.154313
11	13.651733	0.2006880	1.0277554	3.191524	9.614202	7.507373	2647.066	2.308615
12	13.651734	0.2006880	1.0277553	3.191524	9.614202	7.507352	2647.066	2.308602
13	13.651735	0.2006879	1.0277552	3.191524	9.614202	7.507340	2647.066	2.308594
14	13.651736	0.2006879	1.0277552	3.191524	9.614201	7.507331	2647.066	2.308589
15	13.651737	0.2006878	1.0277551	3.191523	9.614201	7.507326	2647.066	2.308586
16	13.651738	0.2006878	1.0277551	3.191523	9.614201	7.507323	2647.066	2.308584
17	13.651739	0.2006878	1.0277550	3.191523	9.614201	7.507322	2647.066	2.308583
18	13.651740	0.2006877	1.0277549	3.191523	9.614201	7.507321	2647.066	2.308583
19	13.651741	0.2006877	1.0277549	3.191523	9.614201	7.507320	2647.066	2.308582
20	13.651742	0.2006876	1.0277548	3.191523	9.614201	7.507320	2647.066	2.308582
21	13.651743	0.2006876	1.0277547	3.191523	9.614201	7.507320	2647.066	2.308582

	hprt	hx	hxd	impd	inuc	mat	polyam	prpps
1	3.669760	0.04730928	1.191281	1.595762	2.642505	14.98849	1.007991	20.88492
2	3.684109	0.04732034	1.191443	1.595750	2.642393	14.98850	1.007991	20.88278
3	3.684104	0.04731730	1.191398	1.595751	2.642401	14.98850	1.007991	20.88275
4	3.684049	0.04731482	1.191362	1.595751	2.642409	14.98850	1.007991	20.88274
5	3.684001	0.04731287	1.191333	1.595752	2.642416	14.98850	1.007991	20.88274
6	3.683961	0.04731135	1.191311	1.595753	2.642422	14.98850	1.007991	20.88273
7	3.683929	0.04731017	1.191294	1.595754	2.642427	14.98850	1.007991	20.88273
8	3.683904	0.04730928	1.191281	1.595754	2.642432	14.98850	1.007991	20.88273
9	3.683883	0.04730860	1.191271	1.595755	2.642437	14.98850	1.007991	20.88273
10	3.683868	0.04730810	1.191264	1.595755	2.642441	14.98850	1.007991	20.88273
11	7.367707	0.09461539	2.382516	3.191511	5.284890	29.97699	2.015983	41.76545
12	7.367676	0.09461462	2.382504	3.191513	5.284902	29.97699	2.015983	41.76545
13	7.367658	0.09461434	2.382500	3.191514	5.284912	29.97699	2.015983	41.76545
14	7.367646	0.09461425	2.382499	3.191515	5.284921	29.97699	2.015983	41.76545
15	7.367640	0.09461435	2.382500	3.191516	5.284929	29.97699	2.015983	41.76545
16	7.367638	0.09461456	2.382503	3.191517	5.284936	29.97699	2.015983	41.76545
17	7.367638	0.09461483	2.382507	3.191518	5.284943	29.97699	2.015983	41.76545
18	7.367639	0.09461512	2.382512	3.191519	5.284948	29.97699	2.015983	41.76545
19	7.367641	0.09461540	2.382516	3.191519	5.284953	29.97699	2.015983	41.76545
20	7.367642	0.09461567	2.382520	3.191520	5.284958	29.97699	2.015983	41.76545
21	7.367644	0.09461592	2.382523	3.191520	5.284962	29.97699	2.015983	41.76545

	pyr	rnaa	rnag	trans	ua	x	xd	R5P	Pi
1	9.99989	1985.551	1323.605	13.98050	2.314825	0.03071716	2.314841	18	1400
2	10.04334	1985.551	1323.605	13.98050	2.314828	0.03072109	2.314923	18	1400
3	10.04368	1985.551	1323.605	13.98050	2.314834	0.03072380	2.314979	18	1400
4	10.04380	1985.550	1323.605	13.98050	2.314842	0.03072494	2.315002	18	1400
5	10.04389	1985.550	1323.605	13.98050	2.314850	0.03072508	2.315005	18	1400

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

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

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

```
   time      PRPP       IMP        SAMP        ATP      SAM          Ade
1   -10  5.000000  98.26340 0.198189000 2475.35000 3.991870 0.9847300000
2    -9  5.017097  98.25819 0.198184839 2475.35234 3.991870 0.9849150719
3    -8  5.017231  98.25855 0.198185337 2475.35377 3.991870 0.9848325423
4    -7  5.017280  98.25890 0.198185738 2475.35440 3.991871 0.9847893888
5    -6  5.017315  98.25922 0.198186049 2475.35459 3.991871 0.9847674154
6    -5  5.017341  98.25951 0.198186302 2475.35458 3.991871 0.9847553831
7    -4  5.017360  98.25977 0.198186517 2475.35449 3.991871 0.9847479991
8    -3  5.017375  98.26000 0.198186702 2475.35438 3.991871 0.9847432878
9    -2  5.017386  98.26020 0.198186865 2475.35426 3.991871 0.9847401086
10   -1  5.017395  98.26039 0.198187011 2475.35415 3.991870 0.9847378781
11    0  5.017401  98.26056 0.198187143 2475.35388 3.991870 0.9847361680
12    1  4.942532  97.64982 0.176888021 2097.34855 3.897049 0.8013941149
13    2  5.263281  96.43286 0.156424689 1747.81132 3.757779 0.6111148919
14    3  5.678426  94.79494 0.136079555 1418.61369 3.604306 0.4334451343
15    4  6.207959  92.84139 0.115207395 1106.99434 3.431282 0.2850700703
16    5  6.906082  90.75058 0.093546041  813.84695 3.229754 0.1708405090
17    6  7.882141  88.89321 0.071072057  543.51880 2.985496 0.0889365122
18    7  9.370363  88.20399 0.048063715  305.51368 2.672649 0.0360755833
19    8 11.954152  91.78347 0.025759482  120.34109 2.240165 0.0088246789
20    9 16.535108 113.03875 0.010344786   28.62137 1.668577 0.0010455917
21   10 19.417926 167.86461 0.007564066   14.10887 1.380950 0.0003501161
       XMP       GTP     dATP     dGTP      RNA      DNA       HX       Xa
1  24.79300  410.2230 6.014130 3.025810 28680.50 5179.340 9.5178500 5.059410
2  24.79299  410.2223 6.014135 3.025813 28680.50 5179.340 9.5198361 5.059734
```

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

```
5  0.9980919 1985.622  8.003053  8.003053 0.2004512   2.402911 0.1008504
6  0.9980853 1985.622  8.003064  8.003063 0.2004512   2.402935 0.1008504
7  0.9980816 1985.622  8.003072  8.003072 0.2004512   2.402953 0.1008504
8  0.9980795 1985.622  8.003080  8.003080 0.2004512   2.402967 0.1008504
9  0.9980783 1985.622  8.003087  8.003087 0.2004513   2.402977 0.1008504
10 0.9980775 1985.622  8.003093  8.003093 0.2004513   2.402985 0.1008504
11 1.0978846 2184.185  8.803409  8.803409 0.2204964   2.643290 0.1109354
12 1.0660070 2173.664  9.186490  9.207377 0.2204399   2.660299 0.1109561
13 1.0386327 2172.109  9.673546  9.693799 0.2202685   3.119270 0.1110638
14 0.9852818 2173.695 10.275909 10.296405 0.2199535   3.763921 0.1112884
15 0.9175062 2174.525 11.030531 11.051698 0.2194628   4.699088 0.1116437
16 0.8430669 2171.337 12.022671 12.044843 0.2187660   6.155691 0.1121430
17 0.7624260 2160.053 13.442904 13.465722 0.2178266   8.678945 0.1128056
18 0.6698860 2133.287 15.779704 15.802348 0.2165890  13.820582 0.1136629
19 0.5545486 2074.276 20.629994 20.650762 0.2149506  27.528781 0.1147714
20 0.4155372 1973.614 32.743065 32.750652 0.2127414  71.998777 0.1162378
21 0.3490630 1948.005 47.037441 47.038307 0.2100987 111.817126 0.1181374
       dnaa     dnag     gdna     gdrnr      gmpr      gmps      gnuc     gprt
1  10.03756 6.826370 6.825859 0.1003440 0.5138721 1.5957628  4.807078 3.738009
2  10.03756 6.826370 6.825863 0.1003438 0.5138758 1.5957629  4.807071 3.753992
3  10.03756 6.826371 6.825864 0.1003439 0.5138768 1.5957629  4.807085 3.753944
4  10.03756 6.826371 6.825864 0.1003440 0.5138774 1.5957628  4.807093 3.753867
5  10.03756 6.826371 6.825865 0.1003440 0.5138776 1.5957627  4.807097 3.753812
6  10.03756 6.826371 6.825865 0.1003440 0.5138777 1.5957626  4.807099 3.753773
7  10.03756 6.826372 6.825865 0.1003440 0.5138778 1.5957625  4.807100 3.753744
8  10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957624  4.807100 3.753723
9  10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957623  4.807101 3.753708
10 10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957622  4.807101 3.753696
11 11.04132 7.509010 7.508453 0.1103784 0.5652655 1.7553383  5.287811 4.129056
12 11.04132 7.509010 7.508106 0.1115850 0.5885785 1.7174249  5.415894 4.041125
13 11.04132 7.509009 7.508058 0.1145702 0.6300674 1.6773472  5.740188 4.166225
14 11.04132 7.509008 7.508551 0.1186844 0.6855959 1.6333970  6.201440 4.300262
15 11.04132 7.509010 7.509405 0.1236232 0.7541371 1.5835068  6.775281 4.493036
16 11.04133 7.509016 7.510433 0.1292989 0.8371371 1.5246584  7.460412 4.779762
17 11.04134 7.509025 7.511460 0.1357848 0.9389181 1.4517185  8.275391 5.209518
18 11.04136 7.509038 7.512250 0.1433395 1.0690032 1.3546662  9.266173 5.883606
19 11.04138 7.509052 7.512353 0.1525608 1.2490797 1.2122299 10.534606 7.048233
20 11.04140 7.509064 7.511233 0.1644974 1.4935988 1.0223255 12.273114 8.899788
21 11.04142 7.509075 7.511978 0.1777200 1.6420994 0.9422041 14.322641 9.289103
       grna      gua     hprt          hx       hxd     impd     inuc       mat
1  1323.532 1.154277 3.669760 0.047309283 1.1912809 1.595762 2.642505 14.988492
2  1323.532 1.154508 3.684109 0.047320340 1.1914425 1.595750 2.642393 14.988495
3  1323.532 1.154452 3.684104 0.047317303 1.1913981 1.595751 2.642401 14.988496
4  1323.533 1.154411 3.684049 0.047314824 1.1913619 1.595751 2.642409 14.988496
5  1323.533 1.154381 3.684001 0.047312868 1.1913333 1.595752 2.642416 14.988496
6  1323.533 1.154359 3.683961 0.047311346 1.1913111 1.595753 2.642422 14.988496
```

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

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

Clearly, this system has stability sensitivity problems.

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

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

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

```
> summary(curto)

$nSpecies
[1] 18
```

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

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

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

$nStates
[1] 16

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

$nReactions
[1] 37

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

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

```
                                "aadna*dATP^fdnap9*dGTP^fdnap10"
                                                            adrnr
                    "aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10"
                                                             ampd
                           "aampd*ATP^fampd4*GTP^fampd8*Pi^fampd18"
                                                             aprt
                         "aaprt*PRPP^faprt1*ATP^faprt4*Ade^faprt6"
                                                             arna
                                      "aarna*ATP^frnap4*GTP^frnap8"
                                                             asuc
               "aasuc*IMP^fasuc2*ATP^fasuc4*GTP^fasuc8*Pi^fasuc18"
                                                             asli
                                    "aasli*SAMP^fasli3*ATP^fasli4"
                                                             dada
                                           "adada*dATP^fdada9"
                                                              den
        "aden*PRPP^fden1*IMP^fden2*ATP^fden4*GTP^fden8*Pi^fden18"
                                                            dgnuc
                                        "adgnuc*dGTP^fdgnuc10"
                                                             dnaa
                                           "adnaa*DNA^fdnan12"
                                                             dnag
                                           "adnag*DNA^fdnan12"
                                                             gdna
                                    "agdna*dATP^fdnap9*dGTP^fdnap10"
                                                            gdrnr
                    "agdrnr*GTP^fgdrnr8*dATP^fgdrnr9*dGTP^fgdrnr10"
                                                             gmpr
               "agmpr*IMP^fgmpr2*ATP^fgmpr4*XMP^fgmpr7*GTP^fgmpr8"
                                                             gmps
                                    "agmps*ATP^fgmps4*XMP^fgmps7"
                                                             gnuc
                                    "agnuc*GTP^fgnuc8*Pi^fgnuc18"
                                                             gprt
                          "agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15"
                                                             grna
                                    "agrna*ATP^frnap4*GTP^frnap8"
                                                              gua
                                                "agua*Gua^fgua15"
                                                             hprt
                           "ahprt*PRPP^fhprt1*IMP^fhprt2*HX^fhprt13"
                                                               hx
                                                  "ahx*HX^fhx13"
                                                              hxd
                                                "ahxd*HX^fhxd13"
                                                             impd
```

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

$V0
         ada          ade         adna        adrnr         ampd         aprt
2.079467e+00 9.915724e-03 1.003826e+01 2.011595e-01 5.640728e+00 9.963412e-01
        arna         asuc         asli         dada          den        dgnuc
1.985621e+03 8.003186e+00 8.003185e+00 2.004510e-01 2.386351e+00 1.008502e-01
        dnaa         dnag         gdna        gdrnr         gmpr         gmps
1.003756e+01 6.826370e+00 6.825859e+00 1.003440e-01 5.138721e-01 1.595763e+00
        gnuc         gprt         grna          gua         hprt           hx
4.807078e+00 3.738009e+00 1.323532e+03 1.154277e+00 3.669760e+00 4.730928e-02
         hxd         impd         inuc          mat       polyam        prpps
1.191281e+00 1.595762e+00 2.642505e+00 1.498849e+01 1.007991e+00 2.088492e+01
         pyr         rnaa         rnag        trans           ua            x
9.999890e+00 1.985551e+03 1.323605e+03 1.398050e+01 2.314825e+00 3.071716e-02
          xd
2.314841e+00

$globalVec
NULL

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

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

```
Xa       0     0     0     0     0     0     0     0     0    -1    -1
Gua      0     0     0     0     0     0     0     0     0     0     0
UA       0     0     0     0     0     0     0     0    -1     0     1

$nRules
[1] 0

$ruleIDs
NULL

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

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

dnag	14
gdna	15
gdrnr	16
gmpr	17
gmps	18
gnuc	19
gprt	20
grna	21
gua	22
hprt	23
hx	24
hxd	25
impd	26
inuc	27
mat	28
polyam	29
prpps	30
pyr	31
rnaa	32
rnag	33
trans	34
ua	35
x	36
xd	37

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

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

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

> curto

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

$id
[1] "curto"

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

$compartments
$compartments$cell
$compartments$cell$id
[1] "cell"

$compartments$cell$size
[1] 1

$compartments$cell$name
[1] "cell"



$species
$species$PRPP
```

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

$species$PRPP$ic
[1] 5

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

$species$PRPP$bc
[1] FALSE


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

$species$IMP$ic
[1] 98.2634

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

$species$IMP$bc
[1] FALSE


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

$species$SAMP$ic
[1] 0.198189

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

$species$SAMP$bc
[1] FALSE


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

$species$ATP$ic
```

```
[1] 2475.35

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

$species$ATP$bc
[1] FALSE


$species$SAM
$species$SAM$id
[1] "SAM"

$species$SAM$ic
[1] 3.99187

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

$species$SAM$bc
[1] FALSE


$species$Ade
$species$Ade$id
[1] "Ade"

$species$Ade$ic
[1] 0.98473

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

$species$Ade$bc
[1] FALSE


$species$XMP
$species$XMP$id
[1] "XMP"

$species$XMP$ic
[1] 24.793

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

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


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

$species$GTP$ic
[1] 410.223

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

$species$GTP$bc
[1] FALSE


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

$species$dATP$ic
[1] 6.01413

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

$species$dATP$bc
[1] FALSE


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

$species$dGTP$ic
[1] 3.02581

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

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

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

$species$RNA$ic
[1] 28680.5

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

$species$RNA$bc
[1] FALSE


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

$species$DNA$ic
[1] 5179.34

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

$species$DNA$bc
[1] FALSE


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

$species$HX$ic
[1] 9.51785

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

$species$HX$bc
[1] FALSE


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

```
$species$Xa$ic
[1] 5.05941

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

$species$Xa$bc
[1] FALSE


$species$Gua
$species$Gua$id
[1] "Gua"

$species$Gua$ic
[1] 5.50638

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

$species$Gua$bc
[1] FALSE


$species$UA
$species$UA$id
[1] "UA"

$species$UA$ic
[1] 100.293

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

$species$UA$bc
[1] FALSE


$species$R5P
$species$R5P$id
[1] "R5P"

$species$R5P$ic
[1] 18
```

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

$species$R5P$bc
[1] TRUE


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

$species$Pi$ic
[1] 1400

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

$species$Pi$bc
[1] TRUE



$globalParameters
list()

$rules
list()

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

$reactions$ada$reversible
[1] FALSE

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

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

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

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

$reactions$ada$exprLaw
aada * ATP^fada4

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

$reactions$ada$law
function (r, p = NULL)
{
    aada = p["aada"]
    fada4 = p["fada4"]
    ATP = r["ATP"]
    aada * ATP^fada4
}
<environment: 0x3a55dc8>


$reactions$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: 0x2fa2878>


$reactions$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: 0x3989ae0>


$reactions$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: 0x35c0320>


$reactions$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: 0x4076ac8>


$reactions$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: 0x39095c8>


$reactions$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: 0x30a18a0>


$reactions$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: 0x4160ed8>


$reactions$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: 0x36de1a0>


$reactions$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: 0x31351f0>


$reactions$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: 0x36f2510>


$reactions$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: 0x1ebcb80>


$reactions$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: 0x36e7438>


$reactions$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: 0x3229000>


$reactions$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: 0x3942248>


$reactions$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: 0x34fdb68>
```

```
$reactions$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: 0x41c2718>


$reactions$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: 0x371c220>


$reactions$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: 0x3074a58>


$reactions$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: 0x39d4330>


$reactions$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: 0x360e9f0>


$reactions$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: 0x2869910>


$reactions$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: 0x3954418>


$reactions$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: 0x34d1c58>


$reactions$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: 0x41a50c0>


$reactions$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: 0x39d0cf0>


$reactions$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: 0x3609788>


$reactions$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: 0x417e6b8>


$reactions$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: 0x3949378>


$reactions$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: 0x30370a8>


$reactions$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: 0x3a28708>


$reactions$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: 0x3717468>


$reactions$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: 0x306aab0>


$reactions$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: 0x39b85b8>


$reactions$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: 0x2c45c28>
```

```
$reactions$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: 0x391f3d8>


$reactions$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: 0x34e1dd8>



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

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

attr(,"class")
[1] "SBMLR"
```