Quick Intro to SBMLR

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Introduction

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

Model import, export, editing and viewing

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

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

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

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

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

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

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

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

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

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

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

Model simulation

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

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

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

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

	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	5.017305	98.25918	0.1981860	2475.354	3.991871	0.9847786	24.79295
6	-5	5.017330	98.25946	0.1981862	2475.354	3.991871	0.9847637	24.79294
7	-4	5.017350	98.25971	0.1981865	2475.354	3.991871	0.9847540	24.79294
8	-3	5.017366	98.25993	0.1981866	2475.354	3.991871	0.9847477	24.79293
9	-2	5.017378	98.26014	0.1981868	2475.354	3.991871	0.9847433	24.79292
10	-1	5.017388	98.26032	0.1981870	2475.354	3.991871	0.9847403	24.79291
11	0	5.017398	98.26058	0.1981872	2475.354	3.991870	0.9847375	24.79290
12	1	5.017406	98.26085	0.1981874	2475.354	3.991870	0.9847354	24.79289
13	2	5.017412	98.26108	0.1981876	2475.354	3.991870	0.9847341	24.79288
14	3	5.017415	98.26129	0.1981877	2475.354	3.991870	0.9847332	24.79287
15	4	5.017418	98.26147	0.1981879	2475.354	3.991870	0.9847326	24.79287
16	5	5.017419	98.26163	0.1981880	2475.354	3.991870	0.9847322	24.79286
17	6	5.017420	98.26178	0.1981881	2475.354	3.991870	0.9847320	24.79285
18	7	5.017421	98.26191	0.1981882	2475.353	3.991870	0.9847318	24.79285
19	8	5.017421	98.26202	0.1981883	2475.353	3.991870	0.9847317	24.79285
20	9	5.017421	98.26213	0.1981884	2475.353	3.991870	0.9847316	24.79284
21	10	5.017421	98.26222	0.1981885	2475.353	3.991870	0.9847316	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	410.2235	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	410.2246	6.014137	3.025814	28680.49	5179.341	9.518586	5.060012	5.507461
6	410.2248	6.014138	3.025814	28680.49	5179.341	9.518324	5.059988	5.507251
7	410.2250	6.014138	3.025814	28680.49	5179.341	9.518116	5.059942	5.507089
8	410.2250	6.014139	3.025814	28680.49	5179.341	9.517952	5.059885	5.506963
9	410.2251	6.014139	3.025814	28680.49	5179.342	9.517825	5.059824	5.506866
10	410.2251	6.014139	3.025814	28680.49	5179.342	9.517726	5.059763	5.506791
11	410.2251	6.014140	3.025814	28680.49	5179.342	9.517627	5.059677	5.506710
12	410.2251	6.014141	3.025814	28680.49	5179.343	9.517555	5.059586	5.506644
13	410.2251	6.014142	3.025814	28680.49	5179.343	9.517523	5.059521	5.506604
14	410.2251	6.014143	3.025815	28680.49	5179.343	9.517510	5.059474	5.506575
15	410.2251	6.014143	3.025815	28680.49	5179.344	9.517511	5.059440	5.506556
16	410.2251	6.014144	3.025815	28680.49	5179.344	9.517521	5.059418	5.506543
17	410.2251	6.014145	3.025815	28680.49	5179.345	9.517536	5.059403	5.506535
18	410.2251	6.014146	3.025815	28680.49	5179.345	9.517553	5.059394	5.506529
19	410.2251	6.014147	3.025815	28680.49	5179.345	9.517573	5.059390	5.506525
20	410.2251	6.014148	3.025815	28680.49	5179.346	9.517592	5.059389	5.506523
21	410.2251	6.014149	3.025816	28680.49	5179.346	9.517611	5.059390	5.506521

	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	0.009915993	10.03827	0.2011597	5.640735	0.9980994	
6	100.2936	2.079471	0.009915911	10.03827	0.2011597	5.640735	0.9980906	
7	100.2937	2.079471	0.009915857	10.03827	0.2011597	5.640735	0.9980852	
8	100.2938	2.079471	0.009915822	10.03827	0.2011597	5.640735	0.9980820	
9	100.2939	2.079470	0.009915798	10.03827	0.2011597	5.640735	0.9980799	
10	100.2939	2.079470	0.009915781	10.03827	0.2011597	5.640735	0.9980786	
11	100.2940	4.158941	0.019831532	20.07655	0.4023194	11.281469	1.9961551	
12	100.2940	4.158940	0.019831508	20.07655	0.4023193	11.281468	1.9961536	
13	100.2940	4.158940	0.019831494	20.07655	0.4023193	11.281468	1.9961527	
14	100.2939	4.158940	0.019831484	20.07655	0.4023193	11.281468	1.9961522	
15	100.2939	4.158940	0.019831477	20.07655	0.4023193	11.281467	1.9961518	
16	100.2938	4.158940	0.019831473	20.07655	0.4023193	11.281467	1.9961516	
17	100.2938	4.158940	0.019831470	20.07655	0.4023193	11.281467	1.9961514	
18	100.2937	4.158940	0.019831468	20.07656	0.4023193	11.281467	1.9961513	
19	100.2937	4.158940	0.019831467	20.07656	0.4023193	11.281467	1.9961512	
20	100.2936	4.158940	0.019831467	20.07656	0.4023193	11.281467	1.9961512	
21	100.2936	4.158940	0.019831466	20.07656	0.4023193	11.281467	1.9961510	

	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	8.002051	0.2004511	2.402705	0.1008503	10.03756	6.826370
3	1985.621	8.003027	8.003034	0.2004511	2.402830	0.1008504	10.03756	6.826371
4	1985.622	8.003040	8.003040	0.2004512	2.402870	0.1008504	10.03756	6.826371
5	1985.622	8.003051	8.003051	0.2004512	2.402901	0.1008504	10.03756	6.826371
6	1985.622	8.003061	8.003061	0.2004512	2.402925	0.1008504	10.03756	6.826371
7	1985.622	8.003070	8.003070	0.2004512	2.402944	0.1008504	10.03756	6.826372
8	1985.622	8.003078	8.003078	0.2004512	2.402958	0.1008504	10.03756	6.826372
9	1985.622	8.003085	8.003085	0.2004513	2.402970	0.1008504	10.03756	6.826372
10	1985.622	8.003091	8.003091	0.2004513	2.402978	0.1008504	10.03756	6.826372
11	3971.245	16.006199	16.006198	0.4009026	4.805976	0.2017008	20.07513	13.652746
12	3971.245	16.006217	16.006217	0.4009026	4.805991	0.2017008	20.07513	13.652747
13	3971.245	16.006232	16.006232	0.4009027	4.806001	0.2017008	20.07513	13.652748
14	3971.245	16.006246	16.006246	0.4009027	4.806007	0.2017008	20.07513	13.652749
15	3971.245	16.006258	16.006258	0.4009028	4.806011	0.2017008	20.07514	13.652750
16	3971.245	16.006268	16.006268	0.4009029	4.806014	0.2017008	20.07514	13.652751
17	3971.245	16.006278	16.006278	0.4009029	4.806015	0.2017008	20.07514	13.652752
18	3971.245	16.006286	16.006286	0.4009030	4.806016	0.2017008	20.07514	13.652753
19	3971.245	16.006294	16.006294	0.4009030	4.806016	0.2017008	20.07514	13.652754
20	3971.245	16.006301	16.006300	0.4009031	4.806017	0.2017009	20.07514	13.652755
21	3971.245	16.006307	16.006307	0.4009032	4.806016	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	3.753990	1323.532	1.154508
3	6.825864	0.1003439	0.5138767	1.595763	4.807084	3.753956	1323.532	1.154457

4	6.825864	0.1003440	0.5138772	1.595763	4.807091	3.753883	1323.532	1.154419
5	6.825865	0.1003440	0.5138775	1.595763	4.807095	3.753830	1323.533	1.154390
6	6.825865	0.1003440	0.5138776	1.595763	4.807097	3.753791	1323.533	1.154368
7	6.825865	0.1003440	0.5138777	1.595763	4.807099	3.753761	1323.533	1.154351
8	6.825866	0.1003440	0.5138777	1.595762	4.807100	3.753738	1323.533	1.154338
9	6.825866	0.1003440	0.5138777	1.595762	4.807100	3.753720	1323.533	1.154328
10	6.825866	0.1003440	0.5138777	1.595762	4.807100	3.753707	1323.533	1.154320
11	13.651733	0.2006880	1.0277554	3.191524	9.614201	7.507386	2647.066	2.308623
12	13.651734	0.2006879	1.0277553	3.191524	9.614201	7.507364	2647.066	2.308609
13	13.651735	0.2006879	1.0277552	3.191524	9.614201	7.507350	2647.066	2.308600
14	13.651736	0.2006879	1.0277552	3.191524	9.614201	7.507340	2647.066	2.308594
15	13.651737	0.2006878	1.0277551	3.191523	9.614201	7.507334	2647.066	2.308590
16	13.651738	0.2006878	1.0277550	3.191523	9.614201	7.507329	2647.066	2.308588
17	13.651739	0.2006878	1.0277550	3.191523	9.614201	7.507326	2647.066	2.308586
18	13.651740	0.2006877	1.0277549	3.191523	9.614201	7.507324	2647.066	2.308585
19	13.651741	0.2006877	1.0277548	3.191523	9.614201	7.507322	2647.066	2.308584
20	13.651742	0.2006876	1.0277548	3.191523	9.614201	7.507322	2647.066	2.308583
21	13.651743	0.2006876	1.0277547	3.191523	9.614201	7.507320	2647.066	2.308583

	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	3.684107	0.04732034	1.191442	1.595750	2.642393	14.98850	1.007991	20.88278
3	3.684108	0.04731749	1.191401	1.595750	2.642401	14.98850	1.007991	20.88275
4	3.684055	0.04731521	1.191368	1.595751	2.642408	14.98850	1.007991	20.88274
5	3.684011	0.04731338	1.191341	1.595752	2.642415	14.98850	1.007991	20.88274
6	3.683974	0.04731192	1.191320	1.595753	2.642421	14.98850	1.007991	20.88274
7	3.683943	0.04731076	1.191303	1.595753	2.642426	14.98850	1.007991	20.88273
8	3.683918	0.04730985	1.191289	1.595754	2.642431	14.98850	1.007991	20.88273
9	3.683897	0.04730914	1.191279	1.595755	2.642435	14.98850	1.007991	20.88273
10	3.683880	0.04730859	1.191271	1.595755	2.642439	14.98850	1.007991	20.88273
11	7.367723	0.09461608	2.382526	3.191511	5.284889	29.97699	2.015983	41.76545
12	7.367692	0.09461528	2.382514	3.191513	5.284901	29.97699	2.015983	41.76545
13	7.367673	0.09461493	2.382509	3.191514	5.284911	29.97699	2.015983	41.76545
14	7.367660	0.09461478	2.382507	3.191515	5.284920	29.97699	2.015983	41.76545
15	7.367652	0.09461479	2.382507	3.191516	5.284928	29.97699	2.015983	41.76545
16	7.367648	0.09461490	2.382508	3.191517	5.284935	29.97699	2.015983	41.76545
17	7.367645	0.09461506	2.382511	3.191518	5.284941	29.97699	2.015983	41.76545
18	7.367644	0.09461526	2.382514	3.191519	5.284947	29.97699	2.015983	41.76545
19	7.367644	0.09461548	2.382517	3.191519	5.284952	29.97699	2.015983	41.76545
20	7.367645	0.09461569	2.382520	3.191520	5.284956	29.97699	2.015983	41.76545
21	7.367645	0.09461591	2.382523	3.191520	5.284960	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	10.04333	1985.551	1323.605	13.98050	2.314828	0.03072109	2.314923	18	1400
3	10.04367	1985.551	1323.605	13.98050	2.314834	0.03072339	2.314970	18	1400
4	10.04378	1985.550	1323.605	13.98050	2.314842	0.03072430	2.314989	18	1400
5	10.04386	1985.550	1323.605	13.98050	2.314849	0.03072446	2.314992	18	1400

```
6  10.04393 1985.550 1323.605 13.98050 2.314856 0.03072417 2.314986  18 1400
7  10.04398 1985.550 1323.605 13.98050 2.314862 0.03072362 2.314975  18 1400
8  10.04402 1985.550 1323.605 13.98050 2.314867 0.03072293 2.314961  18 1400
9  10.04405 1985.550 1323.605 13.98050 2.314870 0.03072219 2.314945  18 1400
10 10.04407 1985.550 1323.605 13.98050 2.314873 0.03072145 2.314930  18 1400
11 20.08820 3971.101 2647.209 27.96101 4.629752 0.06144079 4.629816  18 1400
12 20.08824 3971.101 2647.209 27.96101 4.629753 0.06143857 4.629770  18 1400
13 20.08827 3971.101 2647.209 27.96101 4.629751 0.06143701 4.629738  18 1400
14 20.08829 3971.101 2647.209 27.96101 4.629747 0.06143586 4.629714  18 1400
15 20.08830 3971.101 2647.209 27.96101 4.629742 0.06143505 4.629697  18 1400
16 20.08831 3971.101 2647.209 27.96101 4.629736 0.06143450 4.629686  18 1400
17 20.08831 3971.101 2647.209 27.96101 4.629731 0.06143414 4.629678  18 1400
18 20.08832 3971.101 2647.209 27.96101 4.629725 0.06143393 4.629674  18 1400
19 20.08832 3971.101 2647.209 27.96101 4.629720 0.06143383 4.629672  18 1400
20 20.08832 3971.101 2647.209 27.96101 4.629716 0.06143380 4.629671  18 1400
21 20.08832 3971.101 2647.209 27.96101 4.629712 0.06143382 4.629672  18 1400
```

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))) # half up, half down, not bu
```

```
   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  5.017305  98.25918 0.198185982 2475.35437 3.991871 0.9847785766
6    -5  5.017330  98.25946 0.198186236 2475.35444 3.991871 0.9847636715
7    -4  5.017350  98.25971 0.198186453 2475.35442 3.991871 0.9847540469
8    -3  5.017366  98.25993 0.198186642 2475.35436 3.991871 0.9847476754
9    -2  5.017378  98.26014 0.198186809 2475.35427 3.991871 0.9847433441
10   -1  5.017388  98.26032 0.198186958 2475.35418 3.991871 0.9847403214
11    0  5.016961  98.26053 0.198186992 2475.23312 3.991870 0.9846764949
12    1  4.942401  97.64959 0.176880749 2097.23023 3.897047 0.8013523855
13    2  5.263437  96.43239 0.156419053 1747.71294 3.757707 0.6110508568
14    3  5.678590  94.79449 0.136075318 1418.52398 3.604262 0.4333798560
15    4  6.208129  92.84101 0.115198668 1106.89998 3.431227 0.2850518194
16    5  6.906375  90.75101 0.093528556  813.76310 3.229679 0.1708280611
17    6  7.882624  88.89673 0.071070578  543.45493 2.985402 0.0889365856
18    7  9.371061  88.21985 0.048073052  305.49504 2.672567 0.0360679390
19    8 11.954147  91.82121 0.025777259  120.34145 2.240231 0.0088248220
20    9 16.536277 113.08028 0.010344746   28.61567 1.668473 0.0010452296
21   10 19.418118 167.90535 0.007563083   14.10820 1.380950 0.0003511046
       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
```

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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  410.2246 6.014137 3.025814 28680.49 5179.341 9.5185863 5.060012
6  24.79294  410.2248 6.014138 3.025814 28680.49 5179.341 9.5183240 5.059988
7  24.79294  410.2250 6.014138 3.025814 28680.49 5179.341 9.5181160 5.059942
8  24.79293  410.2250 6.014139 3.025814 28680.49 5179.341 9.5179523 5.059885
9  24.79292  410.2251 6.014139 3.025814 28680.49 5179.342 9.5178247 5.059824
10 24.79291  410.2251 6.014139 3.025814 28680.49 5179.342 9.5177263 5.059763
11 24.79281  410.2251 6.014140 3.025814 28680.61 5179.342 9.5177827 5.059704
12 24.49241  421.2820 6.012596 3.026379 29048.41 5179.342 9.8443689 5.089147
13 24.22822  449.4137 6.007922 3.029317 29372.01 5179.341 9.6201773 5.150183
14 24.00074  489.7175 5.999329 3.035445 29664.35 5179.341 8.8683142 5.210616
15 23.81304  540.3152 5.985943 3.045136 29930.04 5179.342 7.6658217 5.253890
16 23.67125  601.3589 5.966934 3.058758 30168.13 5179.346 6.1107050 5.268448
17 23.58604  674.7873 5.941307 3.076833 30372.62 5179.352 4.3425834 5.243709
18 23.57664  765.1478 5.907543 3.100221 30530.07 5179.361 2.5830354 5.171267
19 23.68104  882.3734 5.862852 3.130461 30611.65 5179.371 1.1874095 5.052292
20 23.97294 1045.5673 5.802595 3.170459 30562.33 5179.380 0.5831356 4.921128
21 24.46778 1241.2775 5.730512 3.222271 30416.40 5179.387 0.9066264 4.893110
        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   5.507461 100.2935 2.07947056 0.0099159933 10.03827 0.2011597 5.64073524
6   5.507251 100.2936 2.07947062 0.0099159108 10.03827 0.2011597 5.64073527
7   5.507089 100.2937 2.07947060 0.0099158575 10.03827 0.2011597 5.64073518
8   5.506963 100.2938 2.07947055 0.0099158222 10.03827 0.2011597 5.64073502
9   5.506866 100.2939 2.07947048 0.0099157982 10.03827 0.2011597 5.64073484
10  5.506791 100.2939 2.07947040 0.0099157815 10.03827 0.2011597 5.64073466
11  5.506797 100.2940 2.28730894 0.0109069708 11.04210 0.2212746 6.20456537
12  5.892612 100.2963 1.94766351 0.0097385798 11.04159 0.2176900 5.42986266
13  6.367518 100.3093 1.63197387 0.0083894836 11.04152 0.2139877 4.68388084
14  7.064392 100.3355 1.33290373 0.0069449717 11.04224 0.2100272 3.95348524
15  8.050486 100.3720 1.04785775 0.0055157019 11.04350 0.2055882 3.23233551
16  9.340313 100.4134 0.77749974 0.0041619825 11.04501 0.2003262 2.51903108
17 10.921602 100.4519 0.52556426 0.0029066111 11.04652 0.1936384 1.81746042
18 12.746949 100.4782 0.30058772 0.0017693323 11.04769 0.1843228 1.14208943
19 14.684959 100.4821 0.12176431 0.0008157009 11.04784 0.1697373 0.53972406
20 16.448684 100.4569 0.03022895 0.0002523243 11.04619 0.1491211 0.17018125
21 18.788950 100.4120 0.01522315 0.0001384786 11.04729 0.1414423 0.09615466
       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
```

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5  0.9980994 1985.622  8.003051  8.003051 0.2004512   2.402901 0.1008504
6  0.9980906 1985.622  8.003061  8.003061 0.2004512   2.402925 0.1008504
7  0.9980852 1985.622  8.003070  8.003070 0.2004512   2.402944 0.1008504
8  0.9980820 1985.622  8.003078  8.003078 0.2004512   2.402958 0.1008504
9  0.9980799 1985.622  8.003085  8.003085 0.2004513   2.402970 0.1008504
10 0.9980786 1985.622  8.003091  8.003091 0.2004513   2.402978 0.1008504
11 1.0978293 2184.179  8.803511  8.803810 0.2204964   2.642858 0.1109354
12 1.0659994 2173.659  9.186612  9.207496 0.2204398   2.660194 0.1109561
13 1.0386132 2172.111  9.673715  9.693972 0.2202685   3.119481 0.1110638
14 0.9852346 2173.699 10.276122 10.296706 0.2199534   3.764173 0.1112885
15 0.9175373 2174.524 11.030801 11.051764 0.2194626   4.699420 0.1116438
16 0.8431081 2171.335 12.023073 12.043793 0.2187657   6.156327 0.1121432
17 0.7625215 2160.053 13.443617 13.466948 0.2178261   8.680164 0.1128059
18 0.6698372 2133.299 15.781281 15.806303 0.2165882  13.822520 0.1136634
19 0.5545539 2074.293 20.633633 20.664812 0.2149497  27.527708 0.1147721
20 0.4155102 1973.606 32.749742 32.756727 0.2127405  72.010299 0.1162385
21 0.3498170 1948.010 47.042901 47.034389 0.2100978 111.818193 0.1181381
       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 3.753990
3  10.03756 6.826371 6.825864 0.1003439 0.5138767 1.5957629  4.807084 3.753956
4  10.03756 6.826371 6.825864 0.1003440 0.5138772 1.5957628  4.807091 3.753883
5  10.03756 6.826371 6.825865 0.1003440 0.5138775 1.5957627  4.807095 3.753830
6  10.03756 6.826371 6.825865 0.1003440 0.5138776 1.5957626  4.807097 3.753791
7  10.03756 6.826372 6.825865 0.1003440 0.5138777 1.5957625  4.807099 3.753761
8  10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957624  4.807100 3.753738
9  10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957623  4.807100 3.753720
10 10.03756 6.826372 6.825866 0.1003440 0.5138777 1.5957622  4.807100 3.753707
11 11.04132 7.509010 7.508453 0.1103784 0.5652690 1.7553270  5.287811 4.128658
12 11.04132 7.509010 7.508106 0.1115852 0.5885840 1.7174123  5.415911 4.041072
13 11.04132 7.509009 7.508057 0.1145716 0.6300846 1.6773351  5.740339 4.166240
14 11.04132 7.509008 7.508551 0.1186862 0.6856184 1.6333841  6.201646 4.300257
15 11.04132 7.509010 7.509406 0.1236246 0.7541580 1.5834901  6.775453 4.493148
16 11.04133 7.509016 7.510434 0.1293008 0.8371631 1.5246394  7.460643 4.779920
17 11.04134 7.509025 7.511460 0.1357875 0.9389487 1.4516984  8.275726 5.209717
18 11.04136 7.509038 7.512251 0.1433437 1.0690239 1.3546577  9.266733 5.883720
19 11.04138 7.509052 7.512355 0.1525650 1.2490470 1.2122325 10.535206 7.047826
20 11.04140 7.509064 7.511234 0.1645009 1.4935684 1.0223035 12.273620 8.900352
21 11.04142 7.509075 7.511979 0.1777232 1.6420667 0.9422013 14.323128 9.289111
       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 3.684107 0.047320338 1.1914425 1.595750 2.642393 14.988495
3  1323.532 1.154457 3.684108 0.047317495 1.1914009 1.595750 2.642401 14.988496
4  1323.532 1.154419 3.684055 0.047315211 1.1913676 1.595751 2.642408 14.988496
5  1323.533 1.154390 3.684011 0.047313382 1.1913408 1.595752 2.642415 14.988496
6  1323.533 1.154368 3.683974 0.047311922 1.1913195 1.595753 2.642421 14.988496
```

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7  1323.533 1.154351 3.683943 0.047310763 1.1913026 1.595753 2.642426 14.988496
8  1323.533 1.154338 3.683918 0.047309852 1.1912893 1.595754 2.642431 14.988496
9  1323.533 1.154328 3.683897 0.047309142 1.1912789 1.595755 2.642435 14.988496
10 1323.533 1.154320 3.683880 0.047308594 1.1912709 1.595755 2.642439 14.988496
11 1191.177 1.038888 3.315185 0.042578017 1.0721479 1.436181 2.378199 13.489514
12 1185.439 1.074665 3.332717 0.044217662 1.0959193 1.435267 2.366363 13.239355
13 1184.595 1.117132 3.571980 0.043091379 1.0796312 1.431190 2.342736 13.047256
14 1185.461 1.176676 3.791706 0.039337554 1.0240075 1.425053 2.310848 12.830881
15 1185.911 1.256118 3.972828 0.033414203 0.9314716 1.417426 2.272673 12.575665
16 1184.172 1.353007 4.088410 0.025920754 0.8038329 1.408821 2.231650 12.262611
17 1178.019 1.463061 4.087821 0.017680856 0.6437878 1.400074 2.195096 11.857960
18 1163.428 1.580602 3.879533 0.009881238 0.4592944 1.393257 2.181715 11.293346
19 1131.249 1.696507 3.369789 0.004137881 0.2771385 1.395108 2.252679 10.420448
20 1076.337 1.795498 2.843674 0.001865895 0.1745648 1.430490 2.661059  9.330570
21 1062.378 1.918981 2.950049 0.003058758 0.2325599 1.507309 3.650872  9.073327
      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 10.043331 1985.551 1323.605 13.980503 2.314828
3  1.0079913  20.88275 10.043669 1985.551 1323.605 13.980504 2.314834
4  1.0079913  20.88274 10.043779 1985.550 1323.605 13.980504 2.314842
5  1.0079913  20.88274 10.043864 1985.550 1323.605 13.980504 2.314849
6  1.0079913  20.88274 10.043929 1985.550 1323.605 13.980504 2.314856
7  1.0079913  20.88273 10.043980 1985.550 1323.605 13.980504 2.314862
8  1.0079913  20.88273 10.044019 1985.550 1323.605 13.980504 2.314867
9  1.0079913  20.88273 10.044050 1985.550 1323.605 13.980504 2.314870
10 1.0079913  20.88273 10.044074 1985.550 1323.605 13.980504 2.314873
11 0.9071922  18.79492  9.038690 1787.003 1191.249 12.582454 2.083388
12 0.8877742  20.23764  8.868436 1809.919 1206.526 12.483026 2.083495
13 0.8591543  21.86987  9.606340 1830.082 1219.967 12.333936 2.084091
14 0.8275137  23.88637 10.578676 1848.296 1232.109 12.165403 2.085293
15 0.7916715  26.53129 11.846933 1864.851 1243.144 11.969484 2.086972
16 0.7496938  30.24369 13.564179 1879.686 1253.033 11.732747 2.088873
17 0.6984624  35.95931 16.044188 1892.427 1261.527 11.432153 2.090645
18 0.6322316  46.12607 19.985617 1902.237 1268.066 11.022080 2.091855
19 0.5393913  69.24099 27.226664 1907.320 1271.455 10.398572 2.092033
20 0.4137403 129.98786 41.111349 1904.247 1269.406  9.435012 2.090873
21 0.3489800 176.61948 50.416057 1895.155 1263.345  8.864124 2.088809
            x       xd R5P   Pi
1  0.03071716 2.314841  18 1400
2  0.03072109 2.314923  18 1400
3  0.03072339 2.314970  18 1400
4  0.03072430 2.314989  18 1400
5  0.03072446 2.314992  18 1400
6  0.03072417 2.314986  18 1400
7  0.03072362 2.314975  18 1400
8  0.03072293 2.314961  18 1400
```

```
9  0.03072219 2.314945  18 1400
10 0.03072145 2.314930  18 1400
11 0.02764865 2.083423  18 1400
12 0.02797137 2.090083  18 1400
13 0.02864634 2.103833  18 1400
14 0.02932256 2.117375  18 1400
15 0.02981163 2.127028  18 1400
16 0.02997706 2.130268  18 1400
17 0.02969620 2.124760  18 1400
18 0.02888137 2.108565  18 1400
19 0.02756771 2.081744  18 1400
20 0.02615490 2.051844  18 1400
21 0.02585793 2.045410  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=simulate(morr,seq(-20,0,1))
> morr$species$EMTX$ic=1 # bolus of methotrexate to 1 uM
> 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,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

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

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

```
$nRules
[1] 0

$ruleIDs
NULL

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

$reactions
       index
ada        1
ade        2
adna       3
adrnr      4
ampd       5
aprt       6
arna       7
asuc       8
asli       9
dada      10
den       11
dgnuc     12
dnaa      13
dnag      14
gdna      15
gdrnr     16
```

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

	Laws
ada	aada*ATP^fada4
ade	aade*Ade^fade6
adna	aadna*dATP^fdnap9*dGTP^fdnap10
adrnr	aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10
ampd	aampd*ATP^fampd4*GTP^fampd8*Pi^fampd18
aprt	aaprt*PRPP^faprt1*ATP^faprt4*Ade^faprt6
arna	aarna*ATP^frnap4*GTP^frnap8
asuc	aasuc*IMP^fasuc2*ATP^fasuc4*GTP^fasuc8*Pi^fasuc18
asli	aasli*SAMP^fasli3*ATP^fasli4
dada	adada*dATP^fdada9
den	aden*PRPP^fden1*IMP^fden2*ATP^fden4*GTP^fden8*Pi^fden18
dgnuc	adgnuc*dGTP^fdgnuc10
dnaa	adnaa*DNA^fdnan12
dnag	adnag*DNA^fdnan12
gdna	agdna*dATP^fdnap9*dGTP^fdnap10
gdrnr	agdrnr*GTP^fgdrnr8*dATP^fgdrnr9*dGTP^fgdrnr10
gmpr	agmpr*IMP^fgmpr2*ATP^fgmpr4*XMP^fgmpr7*GTP^fgmpr8
gmps	agmps*ATP^fgmps4*XMP^fgmps7
gnuc	agnuc*GTP^fgnuc8*Pi^fgnuc18
gprt	agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15
grna	agrna*ATP^frnap4*GTP^frnap8
gua	agua*Gua^fgua15
hprt	ahprt*PRPP^fhprt1*IMP^fhprt2*HX^fhprt13
hx	ahx*HX^fhx13

```
hxd                                                                  ahxd*HX^fhxd13
impd                                        aimpd*IMP^fimpd2*XMP^fimpd7*GTP^fimpd8
inuc                                                  ainuc*IMP^finuc2*Pi^finuc18
mat                                                      amat*ATP^fmat4*SAM^fmat5
polyam                                                       apolyam*SAM^fpolyam5
prpps  aprpps*PRPP^fprpps1*ATP^fprpps4*GTP^fprpps8*R5P^fprpps17*Pi^fprpps18
pyr                                                            apyr*PRPP^fpyr1
rnaa                                                         arnaa*RNA^frnan11
rnag                                                         arnag*RNA^frnan11
trans                                                       atrans*SAM^ftrans5
ua                                                                aua*UA^fua16
x                                                                   ax*Xa^fx14
xd                                                                 axd*Xa^fxd14
       initialFluxes
ada     2.079467e+00
ade     9.915724e-03
adna    1.003826e+01
adrnr   2.011595e-01
ampd    5.640728e+00
aprt    9.963412e-01
arna    1.985621e+03
asuc    8.003186e+00
asli    8.003185e+00
dada    2.004510e-01
den     2.386351e+00
dgnuc   1.008502e-01
dnaa    1.003756e+01
dnag    6.826370e+00
gdna    6.825859e+00
gdrnr   1.003440e-01
gmpr    5.138721e-01
gmps    1.595763e+00
gnuc    4.807078e+00
gprt    3.738009e+00
grna    1.323532e+03
gua     1.154277e+00
hprt    3.669760e+00
hx      4.730928e-02
hxd     1.191281e+00
impd    1.595762e+00
inuc    2.642505e+00
mat     1.498849e+01
polyam  1.007991e+00
prpps   2.088492e+01
pyr     9.999890e+00
rnaa    1.985551e+03
```

```
rnag    1.323605e+03
trans   1.398050e+01
ua      2.314825e+00
x       3.071716e-02
xd      2.314841e+00
```

> curto

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

$id
[1] "curto"

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

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

$compartments$cell$size
[1] 1



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

$species$PRPP$ic
[1] 5
```

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

$species$PRPP$bc
[1] FALSE


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

$species$IMP$ic
[1] 98.2634

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

$species$IMP$bc
[1] FALSE


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

$species$SAMP$ic
[1] 0.198189

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

$species$SAMP$bc
[1] FALSE


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

$species$ATP$ic
[1] 2475.35

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

$species$ATP$bc
```

```
[1] FALSE


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

$species$SAM$ic
[1] 3.99187

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

$species$SAM$bc
[1] FALSE


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

$species$Ade$ic
[1] 0.98473

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

$species$Ade$bc
[1] FALSE


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

$species$XMP$ic
[1] 24.793

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

$species$XMP$bc
[1] FALSE


$species$GTP
```

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

$species$GTP$ic
[1] 410.223

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

$species$GTP$bc
[1] FALSE


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

$species$dATP$ic
[1] 6.01413

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

$species$dATP$bc
[1] FALSE


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

$species$dGTP$ic
[1] 3.02581

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

$species$dGTP$bc
[1] FALSE


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

$species$RNA$ic
```

```
[1] 28680.5

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

$species$RNA$bc
[1] FALSE


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

$species$DNA$ic
[1] 5179.34

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

$species$DNA$bc
[1] FALSE


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

$species$HX$ic
[1] 9.51785

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

$species$HX$bc
[1] FALSE


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

$species$Xa$ic
[1] 5.05941

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

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


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

$species$Gua$ic
[1] 5.50638

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

$species$Gua$bc
[1] FALSE


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

$species$UA$ic
[1] 100.293

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

$species$UA$bc
[1] FALSE


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

$species$R5P$ic
[1] 18

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

$species$R5P$bc
[1] TRUE
```

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

$species$Pi$ic
[1] 1400

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

$species$Pi$bc
[1] TRUE



$globalParameters
list()

$rules
list()

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

$reactions$ada$reversible
[1] FALSE

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

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

$reactions$ada$parameters
    aada    fada4
0.001062 0.970000

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

```
  <ci>ATP</ci>
  <ci>fada4</ci>
 </apply>
</apply>

$reactions$ada$exprLaw
aada * ATP^fada4

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

$reactions$ada$law
function (r, p = NULL)
{
    aada = p["aada"]
    fada4 = p["fada4"]
    ATP = r["ATP"]
    aada * ATP^fada4
}
<environment: 0x1d90e78>


$reactions$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: 0x217cde0>


$reactions$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: 0x2257aa0>


$reactions$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: 0x2181448>


$reactions$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: 0x1eac6c8>


$reactions$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: 0x1b31fd0>


$reactions$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: 0x828070>


$reactions$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: 0x1b63ef8>
```

```
$reactions$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: 0x22459e8>


$reactions$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: 0x21c5800>


$reactions$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: 0x1da5ad8>


$reactions$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: 0x20453e8>


$reactions$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: 0x223f738>


$reactions$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: 0x21d5560>


$reactions$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: 0x22bd540>


$reactions$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: 0x21f2140>


$reactions$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: 0x225c8e0>


$reactions$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: 0x1f87298>


$reactions$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: 0x1e34300>


$reactions$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: 0x22914e0>


$reactions$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: 0x21b3fc8>


$reactions$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: 0x11c8990>


$reactions$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: 0x22bfce0>


$reactions$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: 0x1e8a628>


$reactions$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: 0x16e74c8>


$reactions$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: 0x222d080>


$reactions$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: 0x20ef7d8>


$reactions$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: 0x29c93f8>


$reactions$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: 0x1e06e68>


$reactions$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: 0x12d0ef0>


$reactions$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: 0x1e18cb8>
```

```
$reactions$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: 0x1814380>
```

```
$reactions$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: 0x229ce38>
```

```
$reactions$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: 0x1e1dc68>


$reactions$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: 0x181b8d8>


$reactions$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: 0x2366b90>


$reactions$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: 0x1ed2080>



$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&amp;apos;s below have been set to the system&amp;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"
```