

Quick Intro to SBMLR

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Introduction

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

Model import, export, editing and viewing

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

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

	index	Laws	initialFluxes
ada	1	aada*ATP ^f ada4	2.079466999
ade	2	aade*Ade ^f ade6	0.009915724
adna	3	aadna*dATP ^f dnap9*dGTP ^f dnap10	10.038261346
adrnr	4	aadrnr*ATP ^f adrnr4*dATP ^f adrnr9*dGTP ^f adrnr10	0.201159500
ampd	5	aampd*ATP ^f fampd4*dGTP ^f fampd8*Pi ^f fampd18	5.640727920
aprt	6	aaprt*PRPP ^f faprt1*ATP ^f faprt4*Ade ^f faprt6	0.998075329

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

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

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

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

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

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

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

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

Model simulation

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

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

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

```
> curto$species$PRPP$ic=5 # 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	gmpr	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	2475.23326	3.991870	0.9846765658
12	1	4.942401	97.64959	0.176880756	2097.23035	3.897047	0.8013524517
13	2	5.263436	96.43239	0.156419060	1747.71306	3.757708	0.6110509229
14	3	5.678590	94.79449	0.136075325	1418.52409	3.604262	0.4333799139
15	4	6.208129	92.84101	0.115198676	1106.90009	3.431227	0.2850518656
16	5	6.906375	90.75101	0.093528564	813.76320	3.229679	0.1708280955
17	6	7.882623	88.89673	0.071070586	543.45502	2.985402	0.0889366092
18	7	9.371061	88.21985	0.048073060	305.49511	2.672567	0.0360679528
19	8	11.954146	91.82121	0.025777266	120.34151	2.240231	0.0088248277
20	9	16.536275	113.08026	0.010344749	28.61568	1.668473	0.0010452303
21	10	19.418117	167.90533	0.007563084	14.10820	1.380950	0.0003511048

	XMP	GTP	dATP	dGTP	RNA	DNA	HX	Xa
1	24.79300	410.2230	6.014130	3.025810	28680.50	5179.340	9.5178500	5.059410
2	24.79299	410.2223	6.014135	3.025813	28680.50	5179.340	9.5198359	5.059734

3	24.79298	410.2235	6.014136	3.025813	28680.49	5179.340	9.5193252	5.059924
4	24.79296	410.2242	6.014137	3.025814	28680.49	5179.341	9.5189149	5.059998
5	24.79295	410.2246	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	9.5177826	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	3.029316	29372.01	5179.341	9.6201774	5.150183
14	24.00074	489.7175	5.999329	3.035445	29664.35	5179.341	8.8683146	5.210616
15	23.81304	540.3152	5.985943	3.045136	29930.04	5179.342	7.6658222	5.253890
16	23.67125	601.3589	5.966934	3.058757	30168.13	5179.346	6.1107056	5.268448
17	23.58604	674.7873	5.941307	3.076833	30372.62	5179.352	4.3425840	5.243709
18	23.57664	765.1477	5.907543	3.100221	30530.07	5179.361	2.5830360	5.171267
19	23.68104	882.3733	5.862852	3.130461	30611.65	5179.371	1.1874099	5.052292
20	23.97294	1045.5672	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	0.9066262	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	2.28730906	0.0109069712	11.04210	0.2212746	6.20456565	
12	5.892612	100.2963	1.94766362	0.0097385803	11.04159	0.2176900	5.42986293	
13	6.367518	100.3093	1.63197398	0.0083894841	11.04152	0.2139877	4.68388110	
14	7.064392	100.3355	1.33290383	0.0069449722	11.04224	0.2100272	3.95348549	
15	8.050486	100.3720	1.04785785	0.0055157024	11.04350	0.2055882	3.23233577	
16	9.340313	100.4134	0.77749983	0.0041619830	11.04501	0.2003262	2.51903133	
17	10.921601	100.4519	0.52556435	0.0029066116	11.04652	0.1936384	1.81746067	
18	12.746948	100.4782	0.30058779	0.0017693327	11.04769	0.1843228	1.14208966	
19	14.684958	100.4821	0.12176436	0.0008157012	11.04784	0.1697373	0.53972425	
20	16.448683	100.4569	0.03022896	0.0002523244	11.04619	0.1491211	0.17018132	
21	18.788949	100.4120	0.01522316	0.0001384787	11.04729	0.1414423	0.09615467	
	aprt	arna	asuc	asli	dada	den	dgnuc	
1	0.9963412	1985.621	8.003186	8.003185	0.2004510	2.386351	0.1008502	
2	0.9981829	1985.621	8.003012	8.002051	0.2004511	2.402705	0.1008503	
3	0.9981402	1985.621	8.003027	8.003034	0.2004511	2.402830	0.1008504	
4	0.9981143	1985.622	8.003040	8.003040	0.2004512	2.402870	0.1008504	

5	0.9980994	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	1.0978294	2184.179	8.803511	8.803810	0.2204964	2.642859	0.1109354
12	1.0659994	2173.659	9.186612	9.207496	0.2204398	2.660194	0.1109561
13	1.0386132	2172.111	9.673715	9.693971	0.2202685	3.119481	0.1110638
14	0.9852346	2173.699	10.276121	10.296706	0.2199534	3.764172	0.1112885
15	0.9175373	2174.524	11.030801	11.051764	0.2194626	4.699419	0.1116438
16	0.8431082	2171.335	12.023073	12.043793	0.2187657	6.156327	0.1121432
17	0.7625216	2160.053	13.443616	13.466947	0.2178261	8.680163	0.1128059
18	0.6698372	2133.299	15.781280	15.806302	0.2165882	13.822517	0.1136634
19	0.5545539	2074.293	20.633630	20.664810	0.2149497	27.527700	0.1147721
20	0.4155102	1973.606	32.749736	32.756722	0.2127405	72.010278	0.1162385
21	0.3498171	1948.010	47.042896	47.034383	0.2100978	111.818184	0.1181381
	dnaa	dnag	gdna	gdrnr	gmp	gmps	gnuc
1	10.03756	6.826370	6.825859	0.1003440	0.5138721	1.5957628	4.807078
2	10.03756	6.826370	6.825863	0.1003438	0.5138758	1.5957629	4.807071
3	10.03756	6.826371	6.825864	0.1003439	0.5138767	1.5957629	4.807084
4	10.03756	6.826371	6.825864	0.1003440	0.5138772	1.5957628	4.807091
5	10.03756	6.826371	6.825865	0.1003440	0.5138775	1.5957627	4.807095
6	10.03756	6.826371	6.825865	0.1003440	0.5138776	1.5957626	4.807097
7	10.03756	6.826372	6.825865	0.1003440	0.5138777	1.5957625	4.807099
8	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957624	4.807100
9	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957623	4.807100
10	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957622	4.807100
11	11.04132	7.509010	7.508453	0.1103784	0.5652690	1.7553270	5.287811
12	11.04132	7.509010	7.508106	0.1115852	0.5885839	1.7174123	5.415911
13	11.04132	7.509009	7.508057	0.1145716	0.6300846	1.6773352	5.740339
14	11.04132	7.509008	7.508551	0.1186862	0.6856183	1.6333841	6.201646
15	11.04132	7.509010	7.509406	0.1236246	0.7541580	1.5834902	6.775453
16	11.04133	7.509016	7.510434	0.1293008	0.8371630	1.5246394	7.460643
17	11.04134	7.509025	7.511460	0.1357875	0.9389486	1.4516985	8.275726
18	11.04136	7.509038	7.512251	0.1433437	1.0690238	1.3546578	9.266732
19	11.04138	7.509052	7.512355	0.1525650	1.2490469	1.2122326	10.535205
20	11.04140	7.509064	7.511234	0.1645009	1.4935683	1.0223036	12.273619
21	11.04142	7.509075	7.511979	0.1777232	1.6420667	0.9422013	14.323127
	grna	gua	hp	hx	hxd	impd	inuc
1	1323.532	1.154277	3.669760	0.047309283	1.1912809	1.595762	2.642505
2	1323.532	1.154508	3.684107	0.047320338	1.1914425	1.595750	2.642393
3	1323.532	1.154457	3.684108	0.047317495	1.1914009	1.595750	2.642401
4	1323.532	1.154419	3.684055	0.047315211	1.1913676	1.595751	2.642408
5	1323.533	1.154390	3.684011	0.047313382	1.1913408	1.595752	2.642415
6	1323.533	1.154368	3.683974	0.047311922	1.1913195	1.595753	2.642421
							mat

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	0.042578016	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	0.043091380	1.0796313	1.431190	2.342736	13.047256
14	1185.461	1.176676	3.791706	0.039337556	1.0240075	1.425053	2.310848	12.830881
15	1185.911	1.256118	3.972828	0.033414206	0.9314716	1.417426	2.272673	12.575665
16	1184.172	1.353007	4.088410	0.025920757	0.8038330	1.408821	2.231650	12.262611
17	1178.019	1.463061	4.087821	0.017680859	0.6437879	1.400074	2.195096	11.857960
18	1163.428	1.580602	3.879533	0.009881240	0.4592945	1.393257	2.181715	11.293347
19	1131.249	1.696507	3.369789	0.004137882	0.2771385	1.395108	2.252679	10.420448
20	1076.337	1.795498	2.843674	0.001865895	0.1745648	1.430490	2.661058	9.330571
21	1062.378	1.918981	2.950049	0.003058757	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	9.038691	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	9.606339	1830.082	1219.967	12.333936	2.084091	
14	0.8275138	23.88637	10.578675	1848.296	1232.109	12.165403	2.085293	
15	0.7916715	26.53128	11.846932	1864.851	1243.144	11.969484	2.086972	
16	0.7496938	30.24369	13.564178	1879.686	1253.033	11.732747	2.088873	
17	0.6984624	35.95931	16.044186	1892.427	1261.527	11.432154	2.090645	
18	0.6322317	46.12606	19.985615	1902.237	1268.066	11.022080	2.091855	
19	0.5393914	69.24097	27.226660	1907.320	1271.455	10.398573	2.092033	
20	0.4137403	129.98784	41.111344	1904.247	1269.406	9.435013	2.090873	
21	0.3489800	176.61947	50.416055	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,DHFRductase,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)
```

```

$Species
[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
  Xa  Gua  UA  R5P  Pi
FALSE FALSE FALSE TRUE TRUE

$nStates
[1] 16

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

$nReactions
[1] 37

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

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

```

"aadna*dATP^fdnap9*dGTP^fdnap10"
 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"
 gprr
 "agprr*PRPP^fgprr1*GTP^fgprr8*Gua^fgprr15"
 grna
 "agrna*ATP^frnap4*GTP^frnap8"
 gua
 "agua*Gua^fgua15"
 hprr
 "ahprr*PRPP^fhprr1*IMP^fhprr2*HX^fhprr13"
 hx
 "ahx*HX^fhx13"
 hxd
 "ahxd*HX^fhxd13"
 impd

```

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

```

\$V0

```

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

```

\$incid

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

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

\$nRules

[1] 0

\$ruleIDs

NULL

\$species

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

\$reactions

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

gmp	17
gmp	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
rnac	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
gmp	agmp*IMP^fgmp2*ATP^fgmp4*XMP^fgmp7*GTP^fgmp8
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	
gpri	3.738009e+00	
grna	1.323532e+03	
gua	1.154277e+00	
hpri	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
"http://www.sbml.org/sbml/level2"
                                level
                                "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>

$reactions$aada$exprLaw
aada * ATP^fada4

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

$reactions$aada$law
function (r, p = NULL)
{
  aada = p["aada"]
  fada4 = p["fada4"]
  ATP = r["ATP"]
  aada * ATP^fada4
}
<environment: 0x0291312c>

$reactions$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: 0x02a3e648>

$reactions$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: 0x024ce100>

$reactions$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"

```

```

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

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

$reactions$adnrn$exprLaw
aadnrn * ATP^fadnrn4 * dATP^fadnrn9 * dGTP^fadnrn10

$reactions$adnrn$strLaw
[1] "aadnrn*ATP^fadnrn4*dATP^fadnrn9*dGTP^fadnrn10"

$reactions$adnrn$law
function (r, p = NULL)
{
  aadnrn = p["aadnrn"]
  fadnrn4 = p["fadnrn4"]
  fadnrn9 = p["fadnrn9"]
  fadnrn10 = p["fadnrn10"]
  ATP = r["ATP"]
  dGTP = r["dGTP"]

```

```

    dATP = r["dATP"]
    aadrnr * ATP^fadrnr4 * dATP^fadrnr9 * dGTP^fadrnr10
  }
<environment: 0x02ae9a00>

```

```

$reactions$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>

$reactions$aampd$exprLaw
aampd * ATP^fampd4 * GTP^fampd8 * Pi^fampd18

$reactions$aampd$strLaw
[1] "aampd*ATP^fampd4*GTP^fampd8*Pi^fampd18"

$reactions$aampd$law
function (r, p = NULL)
{
  aampd = p["aampd"]
  fampd4 = p["fampd4"]
  fampd8 = p["fampd8"]
  fampd18 = p["fampd18"]
  ATP = r["ATP"]
  GTP = r["GTP"]
  Pi = r["Pi"]
  aampd * ATP^fampd4 * GTP^fampd8 * Pi^fampd18
}
<environment: 0x0294d060>

$reactions$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: 0x02b7e5cc>

$reactions$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

```



```

$reactions$aarna$strLaw
[1] "aarna*ATP^frnap4*GTP^frnap8"

$reactions$aarna$law
function (r, p = NULL)
{
  aarna = p["aarna"]
  frnap4 = p["frnap4"]
  frnap8 = p["frnap8"]
  ATP = r["ATP"]
  GTP = r["GTP"]
  aarna * ATP^frnap4 * GTP^frnap8
}
<environment: 0x029256c0>

$reactions$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: 0x02ad7748>

```

```

$reactions$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: 0x0283d0ac>

```

```

$reactions$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: 0x013798a4>

$reactions$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>
          <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: 0x02c10488>

```

```

$reactions$dgnuc
$reactions$dgnuc$id
[1] "dgnuc"

```

```

$reactions$dgnuc$reversible
[1] FALSE

```

```

$reactions$dgnuc$reactants
[1] "dGTP"

```

```

$reactions$dgnuc$products
[1] "Gua"

```

```

$reactions$dgnuc$parameters
  adg nuc fdg nuc10
0.03333 1.00000

```

```

$reactions$dgnuc$mathmlLaw
<apply>
  <times/>
  <ci>adg nuc</ci>
  <apply>
    <power/>
    <ci>dGTP</ci>
    <ci>fdg nuc10</ci>
  </apply>
</apply>

```

```

$reactions$dgnuc$exprLaw
adg nuc * dGTP^fdg nuc10

```

```

$reactions$dgnuc$strLaw
[1] "adg nuc*dGTP^fdg nuc10"

```

```

$reactions$dgnuc$law
function (r, p = NULL)

```

```
{
  adgnuc = p["adgnuc"]
  fdgnuc10 = p["fdgnuc10"]
  dGTP = r["dGTP"]
  adgnuc * dGTP^fdgnuc10
}
<environment: 0x02ae4a94>
```

```
$reactions$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: 0x029dda78>

```

```

$reactions$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: 0x02aca4b8>

```

```

$reactions$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: 0x02961cdc>

```

```

$reactions$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: 0x02902874>

$reactions$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: 0x0290bf1c>

$reactions$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: 0x01ed07dc>

$reactions$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: 0x029d61e8>

```

```

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

```

```

$reactions$gpert$reversible
[1] FALSE

```

```

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

```

```

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

```

```

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

```

```

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

```

```

$reactions$gpert$mathmlLaw
<apply>
  <times/>
  <apply>
    <times/>
    <apply>
      <times/>
      <ci>agprt</ci>
      <apply>
        <power/>
        <ci>PRPP</ci>
        <ci>fgprt1</ci>
      </apply>
    </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fgprt8</ci>
  </apply>
</apply>
<apply>

```

```

    <power/>
    <ci>Gua</ci>
    <ci>fgprt15</ci>
  </apply>
</apply>

$reactions$gpert$exprLaw
agprt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15

$reactions$gpert$strLaw
[1] "agprt*PRPP^fgprt1*GTP^fgprt8*Gua^fgprt15"

$reactions$gpert$law
function (r, p = NULL)
{
  agprt = p["agprt"]
  fgprt1 = p["fgprt1"]
  fgprt8 = p["fgprt8"]
  fgprt15 = p["fgprt15"]
  Gua = r["Gua"]
  PRPP = r["PRPP"]
  GTP = r["GTP"]
  agprt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15
}
<environment: 0x02832d64>

$reactions$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: 0x02c31a94>

$reactions$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: 0x014cce9c>

$reactions$hprt
$reactions$hprt$id
[1] "hprt"

$reactions$hprt$reversible
[1] FALSE

$reactions$hprt$reactants

```

```

[1] "HX"      "PRPP"

$reactions$hpert$modifiers
[1] "IMP"

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

$reactions$hpert$parameters
      ahprt  fhprt1  fhprt2 fhprt13
12.569   1.100  -0.890   0.480

$reactions$hpert$mathmlLaw
<apply>
<times/>
<apply>
<times/>
<apply>
<times/>
<ci>ahprt</ci>
<apply>
<power/>
<ci>PRPP</ci>
<ci>fhprt1</ci>
</apply>
</apply>
<apply>
<power/>
<ci>IMP</ci>
<ci>fhprt2</ci>
</apply>
</apply>
<apply>
<power/>
<ci>HX</ci>
<ci>fhprt13</ci>
</apply>
</apply>

$reactions$hpert$exprLaw
ahprt * PRPP^fhprt1 * IMP^fhprt2 * HX^fhprt13

$reactions$hpert$strLaw
[1] "ahprt*PRPP^fhprt1*IMP^fhprt2*HX^fhprt13"

$reactions$hpert$law

```

```

function (r, p = NULL)
{
  ahprt = p["ahprt"]
  fhprt1 = p["fhprt1"]
  fhprt2 = p["fhprt2"]
  fhprt13 = p["fhprt13"]
  HX = r["HX"]
  PRPP = r["PRPP"]
  IMP = r["IMP"]
  ahprt * PRPP^fhprt1 * IMP^fhprt2 * HX^fhprt13
}
<environment: 0x0290ed2c>

```

```

$reactions$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: 0x01eeaf70>

```

```

$reactions$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: 0x0140a554>

$reactions$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>
  <apply>
    <power/>
    <ci>XMP</ci>
  </apply>

```



```

      <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: 0x0292ebd4>

$reactions$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: 0x02b7986c>

$reactions$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: 0x01aff790>

```

```

$reactions$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: 0x02937e20>

```

```

$reactions$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: 0x013b5c0c>

$reactions$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: 0x01ba7850>

```

```

$reactions$rnaa
$reactions$rnaa$id
[1] "rnaa"

$reactions$rnaa$reversible
[1] FALSE

$reactions$rnaa$reactants
[1] "RNA"

$reactions$rnaa$products
[1] "ATP"

$reactions$rnaa$parameters
  arnaa frnan11
0.06923 1.00000

$reactions$rnaa$mathmlLaw
<apply>
  <times/>
  <ci>arna</ci>
  <apply>
    <power/>
    <ci>RNA</ci>
    <ci>frnan11</ci>
  </apply>
</apply>

$reactions$rnaa$exprLaw
arna * RNA^frnan11

$reactions$rnaa$strLaw
[1] "arna*RNA^frnan11"

$reactions$rnaa$law
function (r, p = NULL)
{
  arna = p["arna"]
  frnan11 = p["frnan11"]
  RNA = r["RNA"]
  arna * RNA^frnan11
}
<environment: 0x02911ab8>

```



```

$reactions$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: 0x029bfb98>

```

```

$reactions$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: 0x01415f98>

$reactions$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>ua</ci>
  <apply>
    <power/>
    <ci>UA</ci>
    <ci>fua16</ci>
  </apply>
</apply>

$reactions$ua$exprLaw
ua * UA^fua16

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

$reactions$ua$law
function (r, p = NULL)
{
  aua = p["aua"]
  fua16 = p["fua16"]
  UA = r["UA"]
  aua * UA^fua16
}
<environment: 0x029f6068>

$reactions$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: 0x02c32424>

$reactions$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: 0x01371a3c>
```

```
$htmlNotes
```

```
<notes>
```

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

```
<p>This is a purine metabolism model that is geared toward studies of gout.</p>
```

```
<p>The model is fully described in Curto et al., MBSC 151 (1998) pp 1-49</p>
```

```
<p>The model uses Generalized Mass Action (GMA;i.e. power law) descriptions of reaction ra
```

```
<p>Such descriptions are local approximations that assume independent substrate binding.</p>
```

```
<p/>
```

```
<p>The de novo purine flux vden= 2.39 is in umole/min/KG, i.e. 2.4*60=144 uM/h if we let e
```

```

    <p>liter of water. Morrison and Allegra (JBC, 1989) have vden at 650 uM/h (model) and 415
    <p>The IC&apos;s below have been set to the system&apos;s steady state.</p>
    <p>The units in this model are micromolar(uM) and minutes.</p>
    <p>A cell volume of 1 is used so that amounts and concentrations are the same thing.</p>
  </body>
</notes>

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

```