

# Quick Intro to SBMLR

Tom Radivoyevitch

May 9, 2023

## 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 <sup>f</sup> ada4	2.079466999
ade	2	aade*Ade <sup>f</sup> ade6	0.009915724
adna	3	aadna*dATP <sup>f</sup> dnap9*dGTP <sup>f</sup> dnap10	10.038261346
adrnr	4	aadrnr*ATP <sup>f</sup> adrnr4*dATP <sup>f</sup> adrnr9*dGTP <sup>f</sup> adrnr10	0.201159500
ampd	5	aampd*ATP <sup>f</sup> fampd4*dGTP <sup>f</sup> fampd8*Pi <sup>f</sup> fampd18	5.640727920
aprt	6	aaprt*PRPP <sup>f</sup> aprt1*ATP <sup>f</sup> aprt4*Ade <sup>f</sup> aprt6	0.998075329

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

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

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

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

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

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

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

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

## Model simulation

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

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

The modulator argument to *sim* is either NULL, a vector of numbers, or a list of interpolation functions (time varying enzyme concentration boundary conditions). The vector and list lengths are equal to the number of reactions; in the vector case reaction rate law amplitude parameters are 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
> sim(curto,(-10):10,modulator=rep(2,37)) # bumpless transfer in concentrations since all V
```

	time	PRPP	IMP	SAMP	ATP	SAM	Ade	XMP
1	-10	5.000000	98.26340	0.1981890	2475.350	3.991870	0.9847300	24.79300
2	-9	5.017097	98.25819	0.1981848	2475.352	3.991870	0.9849151	24.79299
3	-8	5.017231	98.25855	0.1981853	2475.354	3.991870	0.9848325	24.79298
4	-7	5.017280	98.25890	0.1981857	2475.354	3.991871	0.9847894	24.79296
5	-6	5.017315	98.25922	0.1981860	2475.355	3.991871	0.9847674	24.79295
6	-5	5.017341	98.25951	0.1981863	2475.355	3.991871	0.9847554	24.79294
7	-4	5.017360	98.25977	0.1981865	2475.354	3.991871	0.9847480	24.79293
8	-3	5.017375	98.26000	0.1981867	2475.354	3.991871	0.9847433	24.79293
9	-2	5.017386	98.26020	0.1981869	2475.354	3.991871	0.9847401	24.79292
10	-1	5.017395	98.26039	0.1981870	2475.354	3.991870	0.9847379	24.79291
11	0	5.017402	98.26058	0.1981872	2475.354	3.991870	0.9847361	24.79290
12	1	5.017411	98.26086	0.1981874	2475.354	3.991870	0.9847342	24.79289
13	2	5.017415	98.26110	0.1981876	2475.354	3.991870	0.9847331	24.79288
14	3	5.017419	98.26131	0.1981877	2475.354	3.991870	0.9847324	24.79287
15	4	5.017421	98.26150	0.1981879	2475.354	3.991870	0.9847319	24.79286
16	5	5.017422	98.26167	0.1981880	2475.354	3.991870	0.9847317	24.79286
17	6	5.017422	98.26181	0.1981881	2475.353	3.991870	0.9847316	24.79285
18	7	5.017422	98.26194	0.1981882	2475.353	3.991870	0.9847315	24.79285
19	8	5.017422	98.26206	0.1981883	2475.353	3.991870	0.9847315	24.79284
20	9	5.017422	98.26216	0.1981884	2475.353	3.991870	0.9847315	24.79284
21	10	5.017422	98.26226	0.1981885	2475.353	3.991870	0.9847315	24.79284
	GTP	dATP	dGTP	RNA	DNA	HX	Xa	Gua
1	410.2230	6.014130	3.025810	28680.50	5179.340	9.517850	5.059410	5.506380
2	410.2223	6.014135	3.025813	28680.50	5179.340	9.519836	5.059734	5.508591
3	410.2237	6.014136	3.025813	28680.49	5179.340	9.519291	5.059957	5.508056
4	410.2244	6.014137	3.025814	28680.49	5179.341	9.518845	5.060051	5.507660
5	410.2248	6.014137	3.025814	28680.49	5179.341	9.518494	5.060063	5.507373
6	410.2250	6.014138	3.025814	28680.49	5179.341	9.518221	5.060026	5.507162
7	410.2251	6.014138	3.025814	28680.49	5179.341	9.518010	5.059964	5.507004
8	410.2251	6.014139	3.025814	28680.49	5179.341	9.517849	5.059891	5.506887
9	410.2251	6.014139	3.025814	28680.49	5179.342	9.517728	5.059816	5.506798
10	410.2251	6.014139	3.025814	28680.49	5179.342	9.517638	5.059744	5.506731
11	410.2251	6.014140	3.025814	28680.49	5179.342	9.517565	5.059668	5.506674
12	410.2251	6.014141	3.025814	28680.49	5179.342	9.517495	5.059567	5.506611
13	410.2251	6.014142	3.025814	28680.49	5179.343	9.517470	5.059494	5.506575
14	410.2251	6.014142	3.025815	28680.49	5179.343	9.517462	5.059439	5.506549
15	410.2251	6.014143	3.025815	28680.49	5179.344	9.517471	5.059403	5.506534
16	410.2251	6.014144	3.025815	28680.49	5179.344	9.517490	5.059382	5.506526
17	410.2251	6.014145	3.025815	28680.49	5179.344	9.517515	5.059373	5.506522
18	410.2251	6.014146	3.025815	28680.49	5179.345	9.517541	5.059370	5.506520
19	410.2251	6.014147	3.025815	28680.49	5179.345	9.517566	5.059371	5.506519
20	410.2251	6.014148	3.025815	28680.49	5179.346	9.517590	5.059375	5.506519
21	410.2251	6.014148	3.025816	28680.49	5179.346	9.517612	5.059380	5.506518
	UA	ada	ade	adna	adrnr	ampd	aprt	
1	100.2930	2.079467	0.009915724	10.03826	0.2011595	5.640728	0.9963412	

2	100.2931	2.079469	0.009916749	10.03827	0.2011596	5.640732	0.9981831	
3	100.2932	2.079470	0.009916292	10.03827	0.2011597	5.640735	0.9981332	
4	100.2933	2.079471	0.009916053	10.03827	0.2011597	5.640735	0.9981052	
5	100.2935	2.079471	0.009915932	10.03827	0.2011597	5.640736	0.9980919	
6	100.2936	2.079471	0.009915865	10.03827	0.2011597	5.640735	0.9980853	
7	100.2938	2.079471	0.009915824	10.03827	0.2011597	5.640735	0.9980816	
8	100.2939	2.079471	0.009915798	10.03827	0.2011597	5.640735	0.9980795	
9	100.2940	2.079470	0.009915780	10.03827	0.2011597	5.640735	0.9980783	
10	100.2940	2.079470	0.009915768	10.03827	0.2011597	5.640735	0.9980775	
11	100.2941	4.158941	0.019831516	20.07655	0.4023194	11.281469	1.9961538	
12	100.2941	4.158940	0.019831495	20.07655	0.4023193	11.281468	1.9961526	
13	100.2940	4.158940	0.019831483	20.07655	0.4023193	11.281468	1.9961521	
14	100.2940	4.158940	0.019831475	20.07655	0.4023193	11.281467	1.9961516	
15	100.2939	4.158940	0.019831470	20.07655	0.4023193	11.281467	1.9961514	
16	100.2939	4.158940	0.019831467	20.07655	0.4023193	11.281467	1.9961513	
17	100.2938	4.158940	0.019831466	20.07655	0.4023193	11.281467	1.9961512	
18	100.2937	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
19	100.2937	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
20	100.2936	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
21	100.2936	4.158940	0.019831465	20.07656	0.4023193	11.281467	1.9961511	
	arna	asuc	asli	dada	den	dgnuc	dnaa	dnag
1	1985.621	8.003186	8.003185	0.2004510	2.386351	0.1008502	10.03756	6.826370
2	1985.621	8.003012	8.003012	0.2004511	2.402707	0.1008503	10.03756	6.826370
3	1985.621	8.003028	8.003027	0.2004512	2.402833	0.1008504	10.03756	6.826371
4	1985.622	8.003042	8.003041	0.2004512	2.402879	0.1008504	10.03756	6.826371
5	1985.622	8.003053	8.003053	0.2004512	2.402911	0.1008504	10.03756	6.826371
6	1985.622	8.003064	8.003063	0.2004512	2.402935	0.1008504	10.03756	6.826371
7	1985.622	8.003072	8.003072	0.2004512	2.402953	0.1008504	10.03756	6.826372
8	1985.622	8.003080	8.003080	0.2004512	2.402967	0.1008504	10.03756	6.826372
9	1985.622	8.003087	8.003087	0.2004513	2.402977	0.1008504	10.03756	6.826372
10	1985.622	8.003093	8.003093	0.2004513	2.402985	0.1008504	10.03756	6.826372
11	3971.245	16.006199	16.006199	0.4009026	4.805985	0.2017008	20.07513	13.652746
12	3971.245	16.006217	16.006217	0.4009026	4.806000	0.2017008	20.07513	13.652747
13	3971.245	16.006233	16.006233	0.4009027	4.806008	0.2017008	20.07513	13.652748
14	3971.245	16.006247	16.006247	0.4009027	4.806014	0.2017008	20.07513	13.652749
15	3971.245	16.006260	16.006259	0.4009028	4.806017	0.2017008	20.07514	13.652750
16	3971.245	16.006270	16.006270	0.4009028	4.806018	0.2017008	20.07514	13.652751
17	3971.245	16.006280	16.006280	0.4009029	4.806019	0.2017008	20.07514	13.652752
18	3971.245	16.006288	16.006288	0.4009030	4.806018	0.2017008	20.07514	13.652753
19	3971.245	16.006296	16.006296	0.4009030	4.806018	0.2017008	20.07514	13.652754
20	3971.245	16.006303	16.006303	0.4009031	4.806018	0.2017009	20.07514	13.652755
21	3971.245	16.006309	16.006309	0.4009031	4.806017	0.2017009	20.07515	13.652756
	gdna	gdrnr	gmpr	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	3.753992	1323.532	1.154508
3	6.825864	0.1003439	0.5138768	1.595763	4.807085	3.753944	1323.532	1.154452

4	6.825864	0.1003440	0.5138774	1.595763	4.807093	3.753867	1323.533	1.154411
5	6.825865	0.1003440	0.5138776	1.595763	4.807097	3.753812	1323.533	1.154381
6	6.825865	0.1003440	0.5138777	1.595763	4.807099	3.753773	1323.533	1.154359
7	6.825865	0.1003440	0.5138778	1.595762	4.807100	3.753744	1323.533	1.154342
8	6.825866	0.1003440	0.5138777	1.595762	4.807100	3.753723	1323.533	1.154330
9	6.825866	0.1003440	0.5138777	1.595762	4.807101	3.753708	1323.533	1.154320
10	6.825866	0.1003440	0.5138777	1.595762	4.807101	3.753696	1323.533	1.154313
11	13.651733	0.2006880	1.0277554	3.191524	9.614202	7.507373	2647.066	2.308615
12	13.651734	0.2006880	1.0277553	3.191524	9.614202	7.507352	2647.066	2.308602
13	13.651735	0.2006879	1.0277552	3.191524	9.614202	7.507340	2647.066	2.308594
14	13.651736	0.2006879	1.0277552	3.191524	9.614201	7.507331	2647.066	2.308589
15	13.651737	0.2006878	1.0277551	3.191523	9.614201	7.507326	2647.066	2.308586
16	13.651738	0.2006878	1.0277551	3.191523	9.614201	7.507323	2647.066	2.308584
17	13.651739	0.2006878	1.0277550	3.191523	9.614201	7.507322	2647.066	2.308583
18	13.651740	0.2006877	1.0277549	3.191523	9.614201	7.507321	2647.066	2.308583
19	13.651741	0.2006877	1.0277549	3.191523	9.614201	7.507320	2647.066	2.308582
20	13.651742	0.2006876	1.0277548	3.191523	9.614201	7.507320	2647.066	2.308582
21	13.651743	0.2006876	1.0277547	3.191523	9.614201	7.507320	2647.066	2.308582
	hprt	hx	hxd	impd	inuc	mat	polyam	prpps
1	3.669760	0.04730928	1.191281	1.595762	2.642505	14.98849	1.007991	20.88492
2	3.684109	0.04732034	1.191443	1.595750	2.642393	14.98850	1.007991	20.88278
3	3.684104	0.04731730	1.191398	1.595751	2.642401	14.98850	1.007991	20.88275
4	3.684049	0.04731482	1.191362	1.595751	2.642409	14.98850	1.007991	20.88274
5	3.684001	0.04731287	1.191333	1.595752	2.642416	14.98850	1.007991	20.88274
6	3.683961	0.04731135	1.191311	1.595753	2.642422	14.98850	1.007991	20.88273
7	3.683929	0.04731017	1.191294	1.595754	2.642427	14.98850	1.007991	20.88273
8	3.683904	0.04730928	1.191281	1.595754	2.642432	14.98850	1.007991	20.88273
9	3.683883	0.04730860	1.191271	1.595755	2.642437	14.98850	1.007991	20.88273
10	3.683868	0.04730810	1.191264	1.595755	2.642441	14.98850	1.007991	20.88273
11	7.367707	0.09461539	2.382516	3.191511	5.284890	29.97699	2.015983	41.76545
12	7.367676	0.09461462	2.382504	3.191513	5.284902	29.97699	2.015983	41.76545
13	7.367658	0.09461434	2.382500	3.191514	5.284912	29.97699	2.015983	41.76545
14	7.367646	0.09461425	2.382499	3.191515	5.284921	29.97699	2.015983	41.76545
15	7.367640	0.09461435	2.382500	3.191516	5.284929	29.97699	2.015983	41.76545
16	7.367638	0.09461456	2.382503	3.191517	5.284936	29.97699	2.015983	41.76545
17	7.367638	0.09461483	2.382507	3.191518	5.284943	29.97699	2.015983	41.76545
18	7.367639	0.09461512	2.382512	3.191519	5.284948	29.97699	2.015983	41.76545
19	7.367641	0.09461540	2.382516	3.191519	5.284953	29.97699	2.015983	41.76545
20	7.367642	0.09461567	2.382520	3.191520	5.284958	29.97699	2.015983	41.76545
21	7.367644	0.09461592	2.382523	3.191520	5.284962	29.97699	2.015983	41.76545
	pyr	rnaa	rnag	trans	ua	x	xd	R5P Pi
1	9.99989	1985.551	1323.605	13.98050	2.314825	0.03071716	2.314841	18 1400
2	10.04334	1985.551	1323.605	13.98050	2.314828	0.03072109	2.314923	18 1400
3	10.04368	1985.551	1323.605	13.98050	2.314834	0.03072380	2.314979	18 1400
4	10.04380	1985.550	1323.605	13.98050	2.314842	0.03072494	2.315002	18 1400
5	10.04389	1985.550	1323.605	13.98050	2.314850	0.03072508	2.315005	18 1400

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

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

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

	time	PRPP	IMP	SAMP	ATP	SAM	Ade
1	-10	5.000000	98.26340	0.198189000	2475.35000	3.991870	0.9847300000
2	-9	5.017097	98.25819	0.198184839	2475.35234	3.991870	0.9849150719
3	-8	5.017231	98.25855	0.198185337	2475.35377	3.991870	0.9848325423
4	-7	5.017280	98.25890	0.198185738	2475.35440	3.991871	0.9847893888
5	-6	5.017315	98.25922	0.198186049	2475.35459	3.991871	0.9847674154
6	-5	5.017341	98.25951	0.198186302	2475.35458	3.991871	0.9847553831
7	-4	5.017360	98.25977	0.198186517	2475.35449	3.991871	0.9847479991
8	-3	5.017375	98.26000	0.198186702	2475.35438	3.991871	0.9847432878
9	-2	5.017386	98.26020	0.198186865	2475.35426	3.991871	0.9847401086
10	-1	5.017395	98.26039	0.198187011	2475.35415	3.991870	0.9847378781
11	0	5.017397	98.26056	0.198187143	2475.35286	3.991870	0.9847356517
12	1	4.942533	97.64982	0.176887968	2097.34762	3.897048	0.8013936331
13	2	5.263284	96.43285	0.156424698	1747.81075	3.757778	0.6111139256
14	3	5.678428	94.79494	0.136080235	1418.61380	3.604306	0.4334435290
15	4	6.207961	92.84139	0.115208250	1106.99433	3.431282	0.2850691628
16	5	6.906078	90.75055	0.093545253	813.84603	3.229755	0.1708417553
17	6	7.882146	88.89316	0.071071875	543.51760	2.985494	0.0889362455
18	7	9.370365	88.20392	0.048064707	305.51267	2.672648	0.0360754481
19	8	11.954166	91.78362	0.025759447	120.34087	2.240163	0.0088246488
20	9	16.535120	113.03883	0.010344698	28.62122	1.668576	0.0010455856
21	10	19.417921	167.86470	0.007564073	14.10889	1.380951	0.0003501169

  

	XMP	GTP	dATP	dGTP	RNA	DNA	HX	Xa
1	24.79300	410.2230	6.014130	3.025810	28680.50	5179.340	9.5178500	5.059410
2	24.79299	410.2223	6.014135	3.025813	28680.50	5179.340	9.5198361	5.059734

3	24.79298	410.2237	6.014136	3.025813	28680.49	5179.340	9.5192907	5.059957
4	24.79296	410.2244	6.014137	3.025814	28680.49	5179.341	9.5188453	5.060051
5	24.79295	410.2248	6.014137	3.025814	28680.49	5179.341	9.5184941	5.060063
6	24.79294	410.2250	6.014138	3.025814	28680.49	5179.341	9.5182207	5.060026
7	24.79293	410.2251	6.014138	3.025814	28680.49	5179.341	9.5180098	5.059964
8	24.79293	410.2251	6.014139	3.025814	28680.49	5179.341	9.5178489	5.059891
9	24.79292	410.2251	6.014139	3.025814	28680.49	5179.342	9.5177278	5.059816
10	24.79291	410.2251	6.014139	3.025814	28680.49	5179.342	9.5176378	5.059744
11	24.79290	410.2251	6.014140	3.025814	28680.49	5179.342	9.5175735	5.059678
12	24.49250	421.2807	6.012598	3.026378	29048.29	5179.342	9.8442791	5.089136
13	24.22829	449.4008	6.007925	3.029316	29371.93	5179.341	9.6202439	5.150116
14	24.00079	489.7001	5.999332	3.035442	29664.27	5179.341	8.8685351	5.210560
15	23.81308	540.3005	5.985949	3.045132	29929.96	5179.342	7.6661565	5.253872
16	23.67127	601.3383	5.966942	3.058752	30168.06	5179.346	6.1109942	5.268423
17	23.58600	674.7569	5.941320	3.076824	30372.58	5179.352	4.3426489	5.243664
18	23.57648	765.0965	5.907563	3.100206	30530.09	5179.361	2.5826148	5.171134
19	23.68077	882.3180	5.862875	3.130442	30611.69	5179.371	1.1867137	5.052039
20	23.97258	1045.5199	5.802620	3.170440	30562.34	5179.380	0.5824028	4.920735
21	24.46735	1241.2312	5.730538	3.222251	30416.42	5179.387	0.9059292	4.892629
	Gua	UA	ada	ade	adna	adrnr	ampd	
1	5.506380	100.2930	2.07946700	0.0099157243	10.03826	0.2011595	5.64072792	
2	5.508591	100.2931	2.07946890	0.0099167492	10.03827	0.2011596	5.64073245	
3	5.508056	100.2932	2.07947007	0.0099162922	10.03827	0.2011597	5.64073451	
4	5.507660	100.2933	2.07947058	0.0099160532	10.03827	0.2011597	5.64073535	
5	5.507373	100.2935	2.07947074	0.0099159315	10.03827	0.2011597	5.64073555	
6	5.507162	100.2936	2.07947073	0.0099158649	10.03827	0.2011597	5.64073545	
7	5.507004	100.2938	2.07947066	0.0099158240	10.03827	0.2011597	5.64073526	
8	5.506887	100.2939	2.07947057	0.0099157979	10.03827	0.2011597	5.64073503	
9	5.506798	100.2940	2.07947047	0.0099157803	10.03827	0.2011597	5.64073480	
10	5.506731	100.2940	2.07947038	0.0099157679	10.03827	0.2011597	5.64073459	
11	5.506681	100.2940	2.28741626	0.0109073312	11.04210	0.2212756	6.20480547	
12	5.892294	100.2964	1.94776926	0.0097388555	11.04159	0.2176911	5.43010635	
13	6.367460	100.3094	1.63206246	0.0083899599	11.04152	0.2139888	4.68409456	
14	7.064236	100.3355	1.33298560	0.0069455329	11.04224	0.2100283	3.95368973	
15	8.049985	100.3720	1.04794439	0.0055158865	11.04350	0.2055896	3.23255856	
16	9.339801	100.4134	0.77757661	0.0041621660	11.04501	0.2003278	2.51923905	
17	10.921125	100.4519	0.52562305	0.0029066050	11.04652	0.1936400	1.81763056	
18	12.746634	100.4782	0.30060455	0.0017695349	11.04768	0.1843229	1.14214447	
19	14.684297	100.4820	0.12176373	0.0008156921	11.04784	0.1697361	0.53972298	
20	16.447371	100.4567	0.03023464	0.0002523716	11.04619	0.1491230	0.17020791	
21	18.787414	100.4118	0.01522387	0.0001382642	11.04728	0.1414420	0.09615851	
	aprt	arna	asuc	asli	dada	den	dgnuc	
1	0.9963412	1985.621	8.003186	8.003185	0.2004510	2.386351	0.1008502	
2	0.9981831	1985.621	8.003012	8.003012	0.2004511	2.402707	0.1008503	
3	0.9981332	1985.621	8.003028	8.003027	0.2004512	2.402833	0.1008504	
4	0.9981052	1985.622	8.003042	8.003041	0.2004512	2.402879	0.1008504	

5	0.9980919	1985.622	8.003053	8.003053	0.2004512	2.402911	0.1008504	
6	0.9980853	1985.622	8.003064	8.003063	0.2004512	2.402935	0.1008504	
7	0.9980816	1985.622	8.003072	8.003072	0.2004512	2.402953	0.1008504	
8	0.9980795	1985.622	8.003080	8.003080	0.2004512	2.402967	0.1008504	
9	0.9980783	1985.622	8.003087	8.003087	0.2004513	2.402977	0.1008504	
10	0.9980775	1985.622	8.003093	8.003093	0.2004513	2.402985	0.1008504	
11	1.0978841	2184.185	8.803410	8.803412	0.2204964	2.643286	0.1109354	
12	1.0660070	2173.664	9.186491	9.207379	0.2204399	2.660300	0.1109561	
13	1.0386320	2172.109	9.673548	9.693803	0.2202685	3.119273	0.1110638	
14	0.9852792	2173.696	10.275912	10.296455	0.2199535	3.763924	0.1112884	
15	0.9175042	2174.525	11.030534	11.051779	0.2194628	4.699091	0.1116437	
16	0.8430720	2171.337	12.022672	12.044755	0.2187660	6.155685	0.1121430	
17	0.7624259	2160.053	13.442907	13.465716	0.2178266	8.678962	0.1128056	
18	0.6698859	2133.286	15.779711	15.802721	0.2165890	13.820601	0.1136629	
19	0.5545483	2074.276	20.630018	20.650770	0.2149506	27.528850	0.1147714	
20	0.4155373	1973.614	32.743117	32.750539	0.2127414	71.998971	0.1162378	
21	0.3490633	1948.005	47.037445	47.038310	0.2100987	111.817024	0.1181374	
	dnaa	dnag	gdna	gdrnr	gmpr	gmps	gnuc	gprr
1	10.03756	6.826370	6.825859	0.1003440	0.5138721	1.5957628	4.807078	3.738009
2	10.03756	6.826370	6.825863	0.1003438	0.5138758	1.5957629	4.807071	3.753992
3	10.03756	6.826371	6.825864	0.1003439	0.5138768	1.5957629	4.807085	3.753944
4	10.03756	6.826371	6.825864	0.1003440	0.5138774	1.5957628	4.807093	3.753867
5	10.03756	6.826371	6.825865	0.1003440	0.5138776	1.5957627	4.807097	3.753812
6	10.03756	6.826371	6.825865	0.1003440	0.5138777	1.5957626	4.807099	3.753773
7	10.03756	6.826372	6.825865	0.1003440	0.5138778	1.5957625	4.807100	3.753744
8	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957624	4.807100	3.753723
9	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957623	4.807101	3.753708
10	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957622	4.807101	3.753696
11	11.04132	7.509010	7.508453	0.1103784	0.5652655	1.7553382	5.287811	4.129052
12	11.04132	7.509010	7.508106	0.1115850	0.5885786	1.7174248	5.415895	4.041125
13	11.04132	7.509009	7.508058	0.1145702	0.6300676	1.6773472	5.740191	4.166223
14	11.04132	7.509008	7.508551	0.1186845	0.6855966	1.6333971	6.201447	4.300254
15	11.04132	7.509010	7.509405	0.1236232	0.7541376	1.5835068	6.775287	4.493031
16	11.04133	7.509016	7.510433	0.1292989	0.8371373	1.5246582	7.460413	4.779760
17	11.04134	7.509025	7.511460	0.1357848	0.9389183	1.4517181	8.275390	5.209524
18	11.04136	7.509038	7.512250	0.1433395	1.0690037	1.3546657	9.266174	5.883607
19	11.04138	7.509052	7.512353	0.1525608	1.2490801	1.2122296	10.534610	7.048237
20	11.04140	7.509064	7.511233	0.1644975	1.4935997	1.0223249	12.273119	8.899790
21	11.04142	7.509075	7.511978	0.1777200	1.6420997	0.9422042	14.322647	9.289094
	grna	gua	hprr	hx	hxd	impd	inuc	mat
1	1323.532	1.154277	3.669760	0.047309283	1.1912809	1.595762	2.642505	14.988492
2	1323.532	1.154508	3.684109	0.047320340	1.1914425	1.595750	2.642393	14.988495
3	1323.532	1.154452	3.684104	0.047317303	1.1913981	1.595751	2.642401	14.988496
4	1323.533	1.154411	3.684049	0.047314824	1.1913619	1.595751	2.642409	14.988496
5	1323.533	1.154381	3.684001	0.047312868	1.1913333	1.595752	2.642416	14.988496
6	1323.533	1.154359	3.683961	0.047311346	1.1913111	1.595753	2.642422	14.988496



7	1323.533	1.154342	3.683929	0.047310172	1.1912939	1.595754	2.642427	14.988496
8	1323.533	1.154330	3.683904	0.047309277	1.1912809	1.595754	2.642432	14.988496
9	1323.533	1.154320	3.683883	0.047308602	1.1912710	1.595755	2.642437	14.988496
10	1323.533	1.154313	3.683868	0.047308101	1.1912637	1.595755	2.642441	14.988496
11	1191.179	1.038877	3.315467	0.042576969	1.0721326	1.436180	2.378200	13.489645
12	1185.442	1.074636	3.332794	0.044217210	1.0959128	1.435267	2.366367	13.239499
13	1184.594	1.117127	3.571863	0.043091714	1.0796361	1.431192	2.342745	13.047255
14	1185.459	1.176663	3.791616	0.039338651	1.0240241	1.425055	2.310857	12.830949
15	1185.912	1.256079	3.972779	0.033415838	0.9314980	1.417428	2.272680	12.575758
16	1184.173	1.352970	4.088328	0.025922128	0.8038577	1.408822	2.231641	12.262688
17	1178.019	1.463029	4.087725	0.017681155	0.6437941	1.400068	2.195026	11.858013
18	1163.421	1.580582	3.879536	0.009879436	0.4592458	1.393223	2.181400	11.293270
19	1131.239	1.696469	3.370074	0.004135165	0.2770329	1.395027	2.251941	10.420625
20	1076.341	1.795426	2.842667	0.001863269	0.1744222	1.430415	2.660278	9.330588
21	1062.375	1.918902	2.949563	0.003056124	0.2324437	1.507258	3.650165	9.073410
	polyam	prpps	pyr	rnaa	rnag	trans	ua	
1	1.0079912	20.88492	9.999890	1985.551	1323.605	13.980504	2.314825	
2	1.0079911	20.88278	10.043336	1985.551	1323.605	13.980503	2.314828	
3	1.0079913	20.88275	10.043676	1985.551	1323.605	13.980504	2.314834	
4	1.0079913	20.88274	10.043802	1985.550	1323.605	13.980504	2.314842	
5	1.0079914	20.88274	10.043890	1985.550	1323.605	13.980504	2.314850	
6	1.0079914	20.88273	10.043956	1985.550	1323.605	13.980505	2.314858	
7	1.0079914	20.88273	10.044005	1985.550	1323.605	13.980504	2.314864	
8	1.0079913	20.88273	10.044043	1985.550	1323.605	13.980504	2.314870	
9	1.0079913	20.88273	10.044071	1985.550	1323.605	13.980504	2.314874	
10	1.0079913	20.88273	10.044093	1985.550	1323.605	13.980504	2.314877	
11	0.9071922	18.79446	9.039689	1786.995	1191.244	12.582454	2.083391	
12	0.8877746	20.23712	8.868737	1809.912	1206.521	12.483028	2.083497	
13	0.8591688	21.86937	9.605985	1830.077	1219.963	12.334013	2.084094	
14	0.8275229	23.88575	10.578292	1848.292	1232.106	12.165453	2.085294	
15	0.7916830	26.53032	11.846527	1864.846	1243.141	11.969548	2.086972	
16	0.7497096	30.24239	13.563438	1879.682	1253.031	11.732838	2.088873	
17	0.6984819	35.95758	16.042954	1892.425	1261.525	11.432270	2.090646	
18	0.6322490	46.12510	19.983731	1902.238	1268.067	11.022191	2.091854	
19	0.5393767	69.24131	27.226718	1907.322	1271.456	10.398469	2.092030	
20	0.4137632	129.97702	41.107698	1904.248	1269.407	9.435204	2.090866	
21	0.3489803	176.61593	50.415408	1895.156	1263.346	8.864126	2.088798	
	x	xd	R5P	Pi				
1	0.03071716	2.314841	18	1400				
2	0.03072109	2.314923	18	1400				
3	0.03072380	2.314979	18	1400				
4	0.03072494	2.315002	18	1400				
5	0.03072508	2.315005	18	1400				
6	0.03072464	2.314996	18	1400				
7	0.03072389	2.314980	18	1400				
8	0.03072300	2.314962	18	1400				

```

9  0.03072209 2.314943 18 1400
10 0.03072121 2.314925 18 1400
11 0.02764837 2.083418 18 1400
12 0.02797125 2.090080 18 1400
13 0.02864559 2.103818 18 1400
14 0.02932193 2.117362 18 1400
15 0.02981143 2.127024 18 1400
16 0.02997679 2.130262 18 1400
17 0.02969570 2.124750 18 1400
18 0.02887988 2.108536 18 1400
19 0.02756494 2.081687 18 1400
20 0.02615072 2.051754 18 1400
21 0.02585285 2.045300 18 1400

```

Clearly, this system has stability sensitivity problems.

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

```

> morr=readSBML(file.path(system.file(package="SBMLR"), "models/morrison.xml"))
> out1=sim(morr,seq(-20,0,1))
> morr$species$EMTX$ic=1 # bolus of methotrexate to 1 uM
> out2=sim(morr,0:30)
> outs=data.frame(rbind(out1,out2))
> attach(outs)
> par(mfrow=c(3,4))
> plot(time,FH2b,type="l",xlab="Hours")
> plot(time,FH2f,type="l",xlab="Hours")
> plot(time,DHFRf,type="l",xlab="Hours")
> plot(time,DHFRtot,type="l",xlab="Hours")
> plot(time,CHOFH4,type="l",xlab="Hours")
> plot(time,FH4,type="l",xlab="Hours")
> plot(time,CH2FH4,type="l",xlab="Hours")
> plot(time,CH3FH4,type="l",xlab="Hours")
> plot(time,AICARsyn,type="l",xlab="Hours")
> plot(time,MTR,type="l",xlab="Hours")
> plot(time,TYMS,type="l",xlab="Hours")
> #plot(time,EMTX,type="l",xlab="Hours")
> plot(time,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" "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"  
 adnrnr  
 "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	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	hpert	hx
	4.807078e+00	3.738009e+00	1.323532e+03	1.154277e+00	3.669760e+00	4.730928e-02
	hxd	impd	inuc	mat	polyam	prpps
	1.191281e+00	1.595762e+00	2.642505e+00	1.498849e+01	1.007991e+00	2.088492e+01
	pyr	rnaa	rnag	trans	ua	x
	9.999890e+00	1.985551e+03	1.323605e+03	1.398050e+01	2.314825e+00	3.071716e-02
	xd					
	2.314841e+00					

\$globalVec

NULL

\$incid

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

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

Xa	0	0	0	0	0	0	0	0	0	0	-1	-1
Gua	0	0	0	0	0	0	0	0	0	0	0	0
UA	0	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
gprr	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*dGTP~fampd8*Pi~fampd18
aprr	aaprr*PRPP~faprr1*ATP~faprr4*Ade~faprr6
arna	aarna*ATP~frnap4*dGTP~frnap8
asuc	aasuc*IMP~fasuc2*ATP~fasuc4*dGTP~fasuc8*Pi~fasuc18
asli	aasli*SAMP~fasli3*ATP~fasli4
dada	adada*dATP~fdada9
den	aden*PRPP~fden1*IMP~fden2*ATP~fden4*dGTP~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*dGTP~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
"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
```

```
$compartments$cell$name
```

```
[1] "cell"
```

```
$species
```

```
$species$PRPP
```

```

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

$species$PRPP$ic
[1] 5

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

$species$PRPP$bc
[1] FALSE

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

$species$IMP$ic
[1] 98.2634

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

$species$IMP$bc
[1] FALSE

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

$species$SAMP$ic
[1] 0.198189

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

$species$SAMP$bc
[1] FALSE

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

$species$ATP$ic

```

```
[1] 2475.35
```

```
$species$ATP$compartment
```

```
[1] "cell"
```

```
$species$ATP$bc
```

```
[1] FALSE
```

```
$species$SAM
```

```
$species$SAM$id
```

```
[1] "SAM"
```

```
$species$SAM$ic
```

```
[1] 3.99187
```

```
$species$SAM$compartment
```

```
[1] "cell"
```

```
$species$SAM$bc
```

```
[1] FALSE
```

```
$species$Ade
```

```
$species$Ade$id
```

```
[1] "Ade"
```

```
$species$Ade$ic
```

```
[1] 0.98473
```

```
$species$Ade$compartment
```

```
[1] "cell"
```

```
$species$Ade$bc
```

```
[1] FALSE
```

```
$species$XMP
```

```
$species$XMP$id
```

```
[1] "XMP"
```

```
$species$XMP$ic
```

```
[1] 24.793
```

```
$species$XMP$compartment
```

```
[1] "cell"
```

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

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

```
$species$GTP$ic  
[1] 410.223
```

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

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

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

```
$species$dATP$ic  
[1] 6.01413
```

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

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

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

```
$species$dGTP$ic  
[1] 3.02581
```

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

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

```

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

$species$RNA$ic
[1] 28680.5

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

$species$RNA$bc
[1] FALSE

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

$species$DNA$ic
[1] 5179.34

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

$species$DNA$bc
[1] FALSE

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

$species$HX$ic
[1] 9.51785

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

$species$HX$bc
[1] FALSE

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

```

```
$species$Xa$ic
```

```
[1] 5.05941
```

```
$species$Xa$compartment
```

```
[1] "cell"
```

```
$species$Xa$bc
```

```
[1] FALSE
```

```
$species$Gua
```

```
$species$Gua$id
```

```
[1] "Gua"
```

```
$species$Gua$ic
```

```
[1] 5.50638
```

```
$species$Gua$compartment
```

```
[1] "cell"
```

```
$species$Gua$bc
```

```
[1] FALSE
```

```
$species$UA
```

```
$species$UA$id
```

```
[1] "UA"
```

```
$species$UA$ic
```

```
[1] 100.293
```

```
$species$UA$compartment
```

```
[1] "cell"
```

```
$species$UA$bc
```

```
[1] FALSE
```

```
$species$R5P
```

```
$species$R5P$id
```

```
[1] "R5P"
```

```
$species$R5P$ic
```

```
[1] 18
```

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

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

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

```
$species$Pi$ic  
[1] 1400
```

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

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

```
$globalParameters  
list()
```

```
$rules  
list()
```

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

```
$reactions$ada$reversible  
[1] FALSE
```

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

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

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



```

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

$reactions$aada$exprLaw
aada * ATP^fada4

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

$reactions$aada$law
function (r, p = NULL)
{
  aada = p["aada"]
  fada4 = p["fada4"]
  ATP = r["ATP"]
  aada * ATP^fada4
}
<environment: 0x1038cd2b8>

$reactions$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: 0x1039164e8>

$reactions$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: 0x1031359f0>

$reactions$adrnr
$reactions$adrnr$id
[1] "adrnr"

$reactions$adrnr$reversible
[1] FALSE

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

```

```

$reactions$adnrn$modifiers
[1] "dGTP" "dATP"

$reactions$adnrn$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)
{

```

```

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: 0x10317a438>

```

```

$reactions$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>

```

```

    <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: 0x1039217f8>

$reactions$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: 0x103966c28>

```

```

$reactions$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>
</apply>

$reactions$aarna$exprLaw
aarna * ATP^frnap4 * GTP^frnap8

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

$reactions$aarna$law
function (r, p = NULL)
{
  aarna = p["aarna"]
  frnap4 = p["frnap4"]
  frnap8 = p["frnap8"]
  ATP = r["ATP"]
  GTP = r["GTP"]
  aarna * ATP^frnap4 * GTP^frnap8
}
<environment: 0x1027ad678>

$reactions$asuc
$reactions$asuc$id
[1] "asuc"

$reactions$asuc$reversible
[1] FALSE

$reactions$asuc$reactants
[1] "IMP"

$reactions$asuc$modifiers
[1] "ATP" "GTP" "Pi"

$reactions$asuc$products
[1] "SAMP"

$reactions$asuc$parameters
  aasuc  fasuc2  fasuc4  fasuc8  fasuc18
3.5932  0.4000 -0.2400  0.2000 -0.0500

$reactions$asuc$mathmlLaw
<apply>
  <times/>
</apply>

```

```

</times>
<apply>
  <times>
    <apply>
      <times>
        <ci>aasuc</ci>
        <apply>
          <power/>
          <ci>IMP</ci>
          <ci>fasuc2</ci>
        </apply>
      </apply>
    </apply>
    <apply>
      <power/>
      <ci>ATP</ci>
      <ci>fasuc4</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fasuc8</ci>
  </apply>
</apply>
<apply>
  <power/>
  <ci>Pi</ci>
  <ci>fasuc18</ci>
</apply>
</apply>

$reactions$asuc$exprLaw
aasuc * IMP^fasuc2 * ATP^fasuc4 * GTP^fasuc8 * Pi^fasuc18

$reactions$asuc$strLaw
[1] "aasuc*IMP^fasuc2*ATP^fasuc4*GTP^fasuc8*Pi^fasuc18"

$reactions$asuc$law
function (r, p = NULL)
{
  aasuc = p["aasuc"]
  fasuc2 = p["fasuc2"]
  fasuc4 = p["fasuc4"]
  fasuc8 = p["fasuc8"]
  fasuc18 = p["fasuc18"]
  IMP = r["IMP"]

```

```

      ATP = r["ATP"]
      GTP = r["GTP"]
      Pi = r["Pi"]
      aasuc * IMP^fasuc2 * ATP^fasuc4 * GTP^fasuc8 * Pi^fasuc18
    }
<bytecode: 0x131e5eb50>
<environment: 0x10399aaa0>

```

```

$reactions$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>
<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: 0x1039dad08>

$reactions$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: 0x1031ca2b0>

$reactions$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
}
<bytecode: 0x1319ae840>
<environment: 0x10401f388>

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

$reactions$dgnuc$reversible
[1] FALSE

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

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

$reactions$dgnuc$parameters
  adgnc fdgnc10
0.03333 1.00000

$reactions$dgnuc$mathmlLaw
<apply>
  <times/>
  <ci>adgnc</ci>
  <apply>
    <power/>
    <ci>dGTP</ci>
    <ci>fdgnc10</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: 0x104058828>

$reactions$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: 0x104083350>

$reactions$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: 0x1040abf58>

```

```

$reactions$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>
<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: 0x1040de710>

$reactions$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>
  <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: 0x104123158>
```

```
$reactions$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
}
<bytecode: 0x102b906e8>
<environment: 0x10417bee8>

$reactions$gmpr
$reactions$gmpr$id
[1] "gmpr"

$reactions$gmpr$reversible
[1] FALSE

$reactions$gmpr$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: 0x1041b82b0>

```

```

$reactions$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: 0x1041ef2a8>

```

```

$reactions$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>

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

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

$reactions$gpirt$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: 0x104237c80>

$reactions$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: 0x1042737b0>

```

```

$reactions$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: 0x10429ee48>

```

```

$reactions$hpert
$reactions$hpert$id
[1] "hpert"

$reactions$hpert$reversible
[1] FALSE

$reactions$hpert$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: 0x1042dee10>

$reactions$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>

$reactions$h{$exprLaw
ahx * HX^fhx13

$reactions$h{$strLaw
[1] "ahx*HX^fhx13"

$reactions$h{$law
function (r, p = NULL)
{
  ahx = p["ahx"]
  fhx13 = p["fhx13"]
  HX = r["HX"]
  ahx * HX^fhx13
}
<environment: 0x10430ee10>

$reactions$h{$id
$reactions$h{$id
[1] "hxd"

$reactions$h{$reversible
[1] FALSE

$reactions$h{$reactants
[1] "HX"

$reactions$h{$products
[1] "Xa"

$reactions$h{$parameters
  ahxd fhxd13
0.2754 0.6500

$reactions$h{$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: 0x1031e5da8>

$reactions$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: 0x103223de0>

$reactions$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: 0x10436b430>

```

```

$reactions$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: 0x1043a04a8>

$reactions$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: 0x1043cba50>

$reactions$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>
    <apply>
      <power/>
      <ci>PRPP</ci>
      <ci>fprpps1</ci>
    </apply>
  </apply>
  <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fprpps4</ci>
  </apply>
  <apply>
    <power/>
    <ci>GTP</ci>
    <ci>fprpps8</ci>
  </apply>
  <apply>
    <power/>
    <ci>R5P</ci>
    <ci>fprpps17</ci>
  </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"]
aprpss * PRPP^fprpps1 * ATP^fprpps4 * GTP^fprpps8 * R5P^fprpps17 *
  Pi^fprpps18
}
<bytecode: 0x1027aaa28>
<environment: 0x102ce32b8>

$reactions$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: 0x102d1a2e8>

```

```

$reactions$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)
{
  arnaa = p["arnaa"]
  frnan11 = p["frnan11"]
  RNA = r["RNA"]
  arnaa * RNA^frnan11
}
<environment: 0x102d3ef00>

```

```

$reactions$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: 0x102d69b08>

```

```

$reactions$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: 0x102d90790>

```

```

$reactions$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: 0x103a152b8>

```

```

$reactions$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: 0x103a41de0>

```

```

$reactions$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: 0x103a66a68>

```

```
$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] "SBMLR"
```