Quick Intro to SBMLR

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Introduction

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

Model import, export, editing and viewing

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

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

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

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

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

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

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

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

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

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

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

Model simulation

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

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

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

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

	time	PRPP	IMP	SAMP	ATP	SAM	Ade	XMP
1	-10	5.000000	98.26340	0.1981890	2475.350	3.991870	0.9847300	24.79300
2	-9	5.017095	98.25819	0.1981608	2475.352	3.991870	0.9849150	24.79299
3	-8	5.017228	98.25854	0.1981855	2475.354	3.991870	0.9848419	24.79298
4	-7	5.017271	98.25887	0.1981857	2475.354	3.991870	0.9848024	24.79296
5	-6	5.017305	98.25918	0.1981860	2475.354	3.991871	0.9847786	24.79295
6	-5	5.017330	98.25946	0.1981862	2475.354	3.991871	0.9847637	24.79294
7	-4	5.017350	98.25971	0.1981865	2475.354	3.991871	0.9847540	24.79294
8	-3	5.017366	98.25993	0.1981866	2475.354	3.991871	0.9847477	24.79293
9	-2	5.017378	98.26014	0.1981868	2475.354	3.991871	0.9847433	24.79292
10	-1	5.017388	98.26032	0.1981870	2475.354	3.991871	0.9847403	24.79291
11	0	5.017398	98.26058	0.1981872	2475.354	3.991870	0.9847375	24.79290
12	1	5.017406	98.26085	0.1981874	2475.354	3.991870	0.9847354	24.79289
13	2	5.017412	98.26108	0.1981876	2475.354	3.991870	0.9847341	24.79288
14	3	5.017415	98.26129	0.1981877	2475.354	3.991870	0.9847332	24.79287
15	4	5.017418	98.26147	0.1981879	2475.354	3.991870	0.9847326	24.79287
16	5	5.017419	98.26163	0.1981880	2475.354	3.991870	0.9847322	24.79286
17	6	5.017420	98.26178	0.1981881	2475.354	3.991870	0.9847320	24.79285
18	7	5.017421	98.26191	0.1981882	2475.353	3.991870	0.9847318	24.79285
19	8	5.017421	98.26202	0.1981883	2475.353	3.991870	0.9847317	24.79285
20	9	5.017421	98.26213	0.1981884	2475.353	3.991870	0.9847316	24.79284
21	10	5.017421	98.26222	0.1981885	2475.353	3.991870	0.9847316	24.79284

	GTP	dATP	dGTP	RNA	DNA	HX	Xa	Gua
1	410.2230	6.014130	3.025810	28680.50	5179.340	9.517850	5.059410	5.506380
2	410.2223	6.014135	3.025813	28680.50	5179.340	9.519836	5.059734	5.508591
3	410.2235	6.014136	3.025813	28680.49	5179.340	9.519325	5.059924	5.508098
4	410.2242	6.014137	3.025814	28680.49	5179.341	9.518915	5.059998	5.507735
5	410.2246	6.014137	3.025814	28680.49	5179.341	9.518586	5.060012	5.507461
6	410.2248	6.014138	3.025814	28680.49	5179.341	9.518324	5.059988	5.507251
7	410.2250	6.014138	3.025814	28680.49	5179.341	9.518116	5.059942	5.507089
8	410.2250	6.014139	3.025814	28680.49	5179.341	9.517952	5.059885	5.506963
9	410.2251	6.014139	3.025814	28680.49	5179.342	9.517825	5.059824	5.506866
10	410.2251	6.014139	3.025814	28680.49	5179.342	9.517726	5.059763	5.506791
11	410.2251	6.014140	3.025814	28680.49	5179.342	9.517627	5.059677	5.506710
12	410.2251	6.014141	3.025814	28680.49	5179.343	9.517555	5.059586	5.506644
13	410.2251	6.014142	3.025814	28680.49	5179.343	9.517523	5.059521	5.506604
14	410.2251	6.014143	3.025815	28680.49	5179.343	9.517510	5.059474	5.506575
15	410.2251	6.014143	3.025815	28680.49	5179.344	9.517511	5.059440	5.506556
16	410.2251	6.014144	3.025815	28680.49	5179.344	9.517521	5.059418	5.506543
17	410.2251	6.014145	3.025815	28680.49	5179.345	9.517536	5.059403	5.506535
18	410.2251	6.014146	3.025815	28680.49	5179.345	9.517553	5.059394	5.506529
19	410.2251	6.014147	3.025815	28680.49	5179.345	9.517573	5.059390	5.506525
20	410.2251	6.014148	3.025815	28680.49	5179.346	9.517592	5.059389	5.506523
21	410.2251	6.014149	3.025816	28680.49	5179.346	9.517611	5.059390	5.506521

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

2	100.2931	2.079469	0.009916749	10.03827	0.2011596	5.640732	0.9981829
3	100.2932	2.079470	0.009916344	10.03827	0.2011597	5.640734	0.9981402
4	100.2933	2.079470	0.009916125	10.03827	0.2011597	5.640735	0.9981143
5	100.2935	2.079471	0.009915993	10.03827	0.2011597	5.640735	0.9980994
6	100.2936	2.079471	0.009915911	10.03827	0.2011597	5.640735	0.9980906
7	100.2937	2.079471	0.009915857	10.03827	0.2011597	5.640735	0.9980852
8	100.2938	2.079471	0.009915822	10.03827	0.2011597	5.640735	0.9980820
9	100.2939	2.079470	0.009915798	10.03827	0.2011597	5.640735	0.9980799
10	100.2939	2.079470	0.009915781	10.03827	0.2011597	5.640735	0.9980786
11	100.2940	4.158941	0.019831532	20.07655	0.4023194	11.281469	1.9961551
12	100.2940	4.158940	0.019831508	20.07655	0.4023193	11.281468	1.9961536
13	100.2940	4.158940	0.019831494	20.07655	0.4023193	11.281468	1.9961527
14	100.2939	4.158940	0.019831484	20.07655	0.4023193	11.281468	1.9961522
15	100.2939	4.158940	0.019831477	20.07655	0.4023193	11.281467	1.9961518
16	100.2938	4.158940	0.019831473	20.07655	0.4023193	11.281467	1.9961516
17	100.2938	4.158940	0.019831470	20.07655	0.4023193	11.281467	1.9961514
18	100.2937	4.158940	0.019831468	20.07656	0.4023193	11.281467	1.9961513
19	100.2937	4.158940	0.019831467	20.07656	0.4023193	11.281467	1.9961512
20	100.2936	4.158940	0.019831467	20.07656	0.4023193	11.281467	1.9961512
21	100.2936	4.158940	0.019831466	20.07656	0.4023193	11.281467	1.9961510

	arna	asuc	asli	dada	den	dgnuc	dnaa	dnag
1	1985.621	8.003186	8.003185	0.2004510	2.386351	0.1008502	10.03756	6.826370
2	1985.621	8.003012	8.002051	0.2004511	2.402705	0.1008503	10.03756	6.826370
3	1985.621	8.003027	8.003034	0.2004511	2.402830	0.1008504	10.03756	6.826371
4	1985.622	8.003040	8.003040	0.2004512	2.402870	0.1008504	10.03756	6.826371
5	1985.622	8.003051	8.003051	0.2004512	2.402901	0.1008504	10.03756	6.826371
6	1985.622	8.003061	8.003061	0.2004512	2.402925	0.1008504	10.03756	6.826371
7	1985.622	8.003070	8.003070	0.2004512	2.402944	0.1008504	10.03756	6.826372
8	1985.622	8.003078	8.003078	0.2004512	2.402958	0.1008504	10.03756	6.826372
9	1985.622	8.003085	8.003085	0.2004513	2.402970	0.1008504	10.03756	6.826372
10	1985.622	8.003091	8.003091	0.2004513	2.402978	0.1008504	10.03756	6.826372
11	3971.245	16.006199	16.006198	0.4009026	4.805976	0.2017008	20.07513	13.652746
12	3971.245	16.006217	16.006217	0.4009026	4.805991	0.2017008	20.07513	13.652747
13	3971.245	16.006232	16.006232	0.4009027	4.806001	0.2017008	20.07513	13.652748
14	3971.245	16.006246	16.006246	0.4009027	4.806007	0.2017008	20.07513	13.652749
15	3971.245	16.006258	16.006258	0.4009028	4.806011	0.2017008	20.07514	13.652750
16	3971.245	16.006268	16.006268	0.4009029	4.806014	0.2017008	20.07514	13.652751
17	3971.245	16.006278	16.006278	0.4009029	4.806015	0.2017008	20.07514	13.652752
18	3971.245	16.006286	16.006286	0.4009030	4.806016	0.2017008	20.07514	13.652753
19	3971.245	16.006294	16.006294	0.4009030	4.806016	0.2017008	20.07514	13.652754
20	3971.245	16.006301	16.006300	0.4009031	4.806017	0.2017009	20.07514	13.652755
21	3971.245	16.006307	16.006307	0.4009032	4.806016	0.2017009	20.07515	13.652756

	gdna	gdrnr	gmpr	gmps	gnuc	gprt	grna	gua
1	6.825859	0.1003440	0.5138721	1.595763	4.807078	3.738009	1323.532	1.154277
2	6.825863	0.1003438	0.5138758	1.595763	4.807071	3.753990	1323.532	1.154508
3	6.825864	0.1003439	0.5138767	1.595763	4.807084	3.753956	1323.532	1.154457

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

	hprt	hx	hxd	impd	inuc	mat	polyam	prpps
1	3.669760	0.04730928	1.191281	1.595762	2.642505	14.98849	1.007991	20.88492
2	3.684107	0.04732034	1.191442	1.595750	2.642393	14.98850	1.007991	20.88278
3	3.684108	0.04731749	1.191401	1.595750	2.642401	14.98850	1.007991	20.88275
4	3.684055	0.04731521	1.191368	1.595751	2.642408	14.98850	1.007991	20.88274
5	3.684011	0.04731338	1.191341	1.595752	2.642415	14.98850	1.007991	20.88274
6	3.683974	0.04731192	1.191320	1.595753	2.642421	14.98850	1.007991	20.88274
7	3.683943	0.04731076	1.191303	1.595753	2.642426	14.98850	1.007991	20.88273
8	3.683918	0.04730985	1.191289	1.595754	2.642431	14.98850	1.007991	20.88273
9	3.683897	0.04730914	1.191279	1.595755	2.642435	14.98850	1.007991	20.88273
10	3.683880	0.04730859	1.191271	1.595755	2.642439	14.98850	1.007991	20.88273
11	7.367723	0.09461608	2.382526	3.191511	5.284889	29.97699	2.015983	41.76545
12	7.367692	0.09461528	2.382514	3.191513	5.284901	29.97699	2.015983	41.76545
13	7.367673	0.09461493	2.382509	3.191514	5.284911	29.97699	2.015983	41.76545
14	7.367660	0.09461478	2.382507	3.191515	5.284920	29.97699	2.015983	41.76545
15	7.367652	0.09461479	2.382507	3.191516	5.284928	29.97699	2.015983	41.76545
16	7.367648	0.09461490	2.382508	3.191517	5.284935	29.97699	2.015983	41.76545
17	7.367645	0.09461506	2.382511	3.191518	5.284941	29.97699	2.015983	41.76545
18	7.367644	0.09461526	2.382514	3.191519	5.284947	29.97699	2.015983	41.76545
19	7.367644	0.09461548	2.382517	3.191519	5.284952	29.97699	2.015983	41.76545
20	7.367645	0.09461569	2.382520	3.191520	5.284956	29.97699	2.015983	41.76545
21	7.367645	0.09461591	2.382523	3.191520	5.284960	29.97699	2.015983	41.76545

	pyr	rnaa	rnag	trans	ua	x	xd	R5P	Pi
1	9.99989	1985.551	1323.605	13.98050	2.314825	0.03071716	2.314841	18	1400
2	10.04333	1985.551	1323.605	13.98050	2.314828	0.03072109	2.314923	18	1400
3	10.04367	1985.551	1323.605	13.98050	2.314834	0.03072339	2.314970	18	1400
4	10.04378	1985.550	1323.605	13.98050	2.314842	0.03072430	2.314989	18	1400
5	10.04386	1985.550	1323.605	13.98050	2.314849	0.03072446	2.314992	18	1400

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

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

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

```
   time      PRPP       IMP        SAMP        ATP      SAM          Ade
1   -10  5.000000  98.26340 0.198189000 2475.35000 3.991870 0.9847300000
2    -9  5.017095  98.25819 0.198160810 2475.35236 3.991870 0.9849150437
3    -8  5.017228  98.25854 0.198185483 2475.35358 3.991870 0.9848418902
4    -7  5.017271  98.25887 0.198185683 2475.35413 3.991870 0.9848024315
5    -6  5.017305  98.25918 0.198185982 2475.35437 3.991871 0.9847785766
6    -5  5.017330  98.25946 0.198186236 2475.35444 3.991871 0.9847636715
7    -4  5.017350  98.25971 0.198186453 2475.35442 3.991871 0.9847540469
8    -3  5.017366  98.25993 0.198186642 2475.35436 3.991871 0.9847476754
9    -2  5.017378  98.26014 0.198186809 2475.35427 3.991871 0.9847433441
10   -1  5.017388  98.26032 0.198186958 2475.35418 3.991871 0.9847403214
11    0  5.016961  98.26053 0.198186992 2475.23312 3.991870 0.9846764949
12    1  4.942401  97.64959 0.176880749 2097.23023 3.897047 0.8013523855
13    2  5.263437  96.43239 0.156419053 1747.71294 3.757707 0.6110508568
14    3  5.678590  94.79449 0.136075318 1418.52398 3.604262 0.4333798560
15    4  6.208129  92.84101 0.115198668 1106.89998 3.431227 0.2850518194
16    5  6.906375  90.75101 0.093528556  813.76310 3.229679 0.1708280611
17    6  7.882624  88.89673 0.071070578  543.45493 2.985402 0.0889365856
18    7  9.371061  88.21985 0.048073052  305.49504 2.672567 0.0360679390
19    8 11.954147  91.82121 0.025777259  120.34145 2.240231 0.0088248220
20    9 16.536277 113.08028 0.010344746   28.61567 1.668473 0.0010452296
21   10 19.418118 167.90535 0.007563083   14.10820 1.380950 0.0003511046
        XMP       GTP     dATP     dGTP      RNA      DNA        HX       Xa
1  24.79300  410.2230 6.014130 3.025810 28680.50 5179.340 9.5178500 5.059410
2  24.79299  410.2223 6.014135 3.025813 28680.50 5179.340 9.5198359 5.059734
```

3	24.79298	410.2235	6.014136	3.025813	28680.49	5179.340	9.5193252	5.059924
4	24.79296	410.2242	6.014137	3.025814	28680.49	5179.341	9.5189149	5.059998
5	24.79295	410.2246	6.014137	3.025814	28680.49	5179.341	9.5185863	5.060012
6	24.79294	410.2248	6.014138	3.025814	28680.49	5179.341	9.5183240	5.059988
7	24.79294	410.2250	6.014138	3.025814	28680.49	5179.341	9.5181160	5.059942
8	24.79293	410.2250	6.014139	3.025814	28680.49	5179.341	9.5179523	5.059885
9	24.79292	410.2251	6.014139	3.025814	28680.49	5179.342	9.5178247	5.059824
10	24.79291	410.2251	6.014139	3.025814	28680.49	5179.342	9.5177263	5.059763
11	24.79281	410.2251	6.014140	3.025814	28680.61	5179.342	9.5177827	5.059704
12	24.49241	421.2820	6.012596	3.026379	29048.41	5179.342	9.8443689	5.089147
13	24.22822	449.4137	6.007922	3.029317	29372.01	5179.341	9.6201773	5.150183
14	24.00074	489.7175	5.999329	3.035445	29664.35	5179.341	8.8683142	5.210616
15	23.81304	540.3152	5.985943	3.045136	29930.04	5179.342	7.6658217	5.253890
16	23.67125	601.3589	5.966934	3.058758	30168.13	5179.346	6.1107050	5.268448
17	23.58604	674.7873	5.941307	3.076833	30372.62	5179.352	4.3425834	5.243709
18	23.57664	765.1478	5.907543	3.100221	30530.07	5179.361	2.5830354	5.171267
19	23.68104	882.3734	5.862852	3.130461	30611.65	5179.371	1.1874095	5.052292
20	23.97294	1045.5673	5.802595	3.170459	30562.33	5179.380	0.5831356	4.921128
21	24.46778	1241.2775	5.730512	3.222271	30416.40	5179.387	0.9066264	4.893110

	Gua	UA	ada	ade	adna	adrnr	ampd
1	5.506380	100.2930	2.07946700	0.0099157243	10.03826	0.2011595	5.64072792
2	5.508591	100.2931	2.07946892	0.0099167491	10.03827	0.2011596	5.64073249
3	5.508098	100.2932	2.07946992	0.0099163440	10.03827	0.2011597	5.64073423
4	5.507735	100.2933	2.07947037	0.0099161254	10.03827	0.2011597	5.64073496
5	5.507461	100.2935	2.07947056	0.0099159933	10.03827	0.2011597	5.64073524
6	5.507251	100.2936	2.07947062	0.0099159108	10.03827	0.2011597	5.64073527
7	5.507089	100.2937	2.07947060	0.0099158575	10.03827	0.2011597	5.64073518
8	5.506963	100.2938	2.07947055	0.0099158222	10.03827	0.2011597	5.64073502
9	5.506866	100.2939	2.07947048	0.0099157982	10.03827	0.2011597	5.64073484
10	5.506791	100.2939	2.07947040	0.0099157815	10.03827	0.2011597	5.64073466
11	5.506797	100.2940	2.28730894	0.0109069708	11.04210	0.2212746	6.20456537
12	5.892612	100.2963	1.94766351	0.0097385798	11.04159	0.2176900	5.42986266
13	6.367518	100.3093	1.63197387	0.0083894836	11.04152	0.2139877	4.68388084
14	7.064392	100.3355	1.33290373	0.0069449717	11.04224	0.2100272	3.95348524
15	8.050486	100.3720	1.04785775	0.0055157019	11.04350	0.2055882	3.23233551
16	9.340313	100.4134	0.77749974	0.0041619825	11.04501	0.2003262	2.51903108
17	10.921602	100.4519	0.52556426	0.0029066111	11.04652	0.1936384	1.81746042
18	12.746949	100.4782	0.30058772	0.0017693323	11.04769	0.1843228	1.14208943
19	14.684959	100.4821	0.12176431	0.0008157009	11.04784	0.1697373	0.53972406
20	16.448684	100.4569	0.03022895	0.0002523243	11.04619	0.1491211	0.17018125
21	18.788950	100.4120	0.01522315	0.0001384786	11.04729	0.1414423	0.09615466

	aprt	arna	asuc	asli	dada	den	dgnuc
1	0.9963412	1985.621	8.003186	8.003185	0.2004510	2.386351	0.1008502
2	0.9981829	1985.621	8.003012	8.002051	0.2004511	2.402705	0.1008503
3	0.9981402	1985.621	8.003027	8.003034	0.2004511	2.402830	0.1008504
4	0.9981143	1985.622	8.003040	8.003040	0.2004512	2.402870	0.1008504

5	0.9980994	1985.622	8.003051	8.003051	0.2004512	2.402901	0.1008504
6	0.9980906	1985.622	8.003061	8.003061	0.2004512	2.402925	0.1008504
7	0.9980852	1985.622	8.003070	8.003070	0.2004512	2.402944	0.1008504
8	0.9980820	1985.622	8.003078	8.003078	0.2004512	2.402958	0.1008504
9	0.9980799	1985.622	8.003085	8.003085	0.2004513	2.402970	0.1008504
10	0.9980786	1985.622	8.003091	8.003091	0.2004513	2.402978	0.1008504
11	1.0978293	2184.179	8.803511	8.803810	0.2204964	2.642858	0.1109354
12	1.0659994	2173.659	9.186612	9.207496	0.2204398	2.660194	0.1109561
13	1.0386132	2172.111	9.673715	9.693972	0.2202685	3.119481	0.1110638
14	0.9852346	2173.699	10.276122	10.296706	0.2199534	3.764173	0.1112885
15	0.9175373	2174.524	11.030801	11.051764	0.2194626	4.699420	0.1116438
16	0.8431081	2171.335	12.023073	12.043793	0.2187657	6.156327	0.1121432
17	0.7625215	2160.053	13.443617	13.466948	0.2178261	8.680164	0.1128059
18	0.6698372	2133.299	15.781281	15.806303	0.2165882	13.822520	0.1136634
19	0.5545539	2074.293	20.633633	20.664812	0.2149497	27.527708	0.1147721
20	0.4155102	1973.606	32.749742	32.756727	0.2127405	72.010299	0.1162385
21	0.3498170	1948.010	47.042901	47.034389	0.2100978	111.818193	0.1181381

	dnaa	dnag	gdna	gdrnr	gmpr	gmps	gnuc	gprt
1	10.03756	6.826370	6.825859	0.1003440	0.5138721	1.5957628	4.807078	3.738009
2	10.03756	6.826370	6.825863	0.1003438	0.5138758	1.5957629	4.807071	3.753990
3	10.03756	6.826371	6.825864	0.1003439	0.5138767	1.5957629	4.807084	3.753956
4	10.03756	6.826371	6.825864	0.1003440	0.5138772	1.5957628	4.807091	3.753883
5	10.03756	6.826371	6.825865	0.1003440	0.5138775	1.5957627	4.807095	3.753830
6	10.03756	6.826371	6.825865	0.1003440	0.5138776	1.5957626	4.807097	3.753791
7	10.03756	6.826372	6.825865	0.1003440	0.5138777	1.5957625	4.807099	3.753761
8	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957624	4.807100	3.753738
9	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957623	4.807100	3.753720
10	10.03756	6.826372	6.825866	0.1003440	0.5138777	1.5957622	4.807100	3.753707
11	11.04132	7.509010	7.508453	0.1103784	0.5652690	1.7553270	5.287811	4.128658
12	11.04132	7.509010	7.508106	0.1115852	0.5885840	1.7174123	5.415911	4.041072
13	11.04132	7.509009	7.508057	0.1145716	0.6300846	1.6773351	5.740339	4.166240
14	11.04132	7.509008	7.508551	0.1186862	0.6856184	1.6333841	6.201646	4.300257
15	11.04132	7.509010	7.509406	0.1236246	0.7541580	1.5834901	6.775453	4.493148
16	11.04133	7.509016	7.510434	0.1293008	0.8371631	1.5246394	7.460643	4.779920
17	11.04134	7.509025	7.511460	0.1357875	0.9389487	1.4516984	8.275726	5.209717
18	11.04136	7.509038	7.512251	0.1433437	1.0690239	1.3546577	9.266733	5.883720
19	11.04138	7.509052	7.512355	0.1525650	1.2490470	1.2122325	10.535206	7.047826
20	11.04140	7.509064	7.511234	0.1645009	1.4935684	1.0223035	12.273620	8.900352
21	11.04142	7.509075	7.511979	0.1777232	1.6420667	0.9422013	14.323128	9.289111

	grna	gua	hprt	hx	hxd	impd	inuc	mat
1	1323.532	1.154277	3.669760	0.047309283	1.1912809	1.595762	2.642505	14.988492
2	1323.532	1.154508	3.684107	0.047320338	1.1914425	1.595750	2.642393	14.988495
3	1323.532	1.154457	3.684108	0.047317495	1.1914009	1.595750	2.642401	14.988496
4	1323.532	1.154419	3.684055	0.047315211	1.1913676	1.595751	2.642408	14.988496
5	1323.533	1.154390	3.684011	0.047313382	1.1913408	1.595752	2.642415	14.988496
6	1323.533	1.154368	3.683974	0.047311922	1.1913195	1.595753	2.642421	14.988496

7	1323.533	1.154351	3.683943	0.047310763	1.1913026	1.595753	2.642426	14.988496
8	1323.533	1.154338	3.683918	0.047309852	1.1912893	1.595754	2.642431	14.988496
9	1323.533	1.154328	3.683897	0.047309142	1.1912789	1.595755	2.642435	14.988496
10	1323.533	1.154320	3.683880	0.047308594	1.1912709	1.595755	2.642439	14.988496
11	1191.177	1.038888	3.315185	0.042578017	1.0721479	1.436181	2.378199	13.489514
12	1185.439	1.074665	3.332717	0.044217662	1.0959193	1.435267	2.366363	13.239355
13	1184.595	1.117132	3.571980	0.043091379	1.0796312	1.431190	2.342736	13.047256
14	1185.461	1.176676	3.791706	0.039337554	1.0240075	1.425053	2.310848	12.830881
15	1185.911	1.256118	3.972828	0.033414203	0.9314716	1.417426	2.272673	12.575665
16	1184.172	1.353007	4.088410	0.025920754	0.8038329	1.408821	2.231650	12.262611
17	1178.019	1.463061	4.087821	0.017680856	0.6437878	1.400074	2.195096	11.857960
18	1163.428	1.580602	3.879533	0.009881238	0.4592944	1.393257	2.181715	11.293346
19	1131.249	1.696507	3.369789	0.004137881	0.2771385	1.395108	2.252679	10.420448
20	1076.337	1.795498	2.843674	0.001865895	0.1745648	1.430490	2.661059	9.330570
21	1062.378	1.918981	2.950049	0.003058758	0.2325599	1.507309	3.650872	9.073327

	polyam	prpps	pyr	rnaa	rnag	trans	ua
1	1.0079912	20.88492	9.999890	1985.551	1323.605	13.980504	2.314825
2	1.0079911	20.88278	10.043331	1985.551	1323.605	13.980503	2.314828
3	1.0079913	20.88275	10.043669	1985.551	1323.605	13.980504	2.314834
4	1.0079913	20.88274	10.043779	1985.550	1323.605	13.980504	2.314842
5	1.0079913	20.88274	10.043864	1985.550	1323.605	13.980504	2.314849
6	1.0079913	20.88274	10.043929	1985.550	1323.605	13.980504	2.314856
7	1.0079913	20.88273	10.043980	1985.550	1323.605	13.980504	2.314862
8	1.0079913	20.88273	10.044019	1985.550	1323.605	13.980504	2.314867
9	1.0079913	20.88273	10.044050	1985.550	1323.605	13.980504	2.314870
10	1.0079913	20.88273	10.044074	1985.550	1323.605	13.980504	2.314873
11	0.9071922	18.79492	9.038690	1787.003	1191.249	12.582454	2.083388
12	0.8877742	20.23764	8.868436	1809.919	1206.526	12.483026	2.083495
13	0.8591543	21.86987	9.606340	1830.082	1219.967	12.333936	2.084091
14	0.8275137	23.88637	10.578676	1848.296	1232.109	12.165403	2.085293
15	0.7916715	26.53129	11.846933	1864.851	1243.144	11.969484	2.086972
16	0.7496938	30.24369	13.564179	1879.686	1253.033	11.732747	2.088873
17	0.6984624	35.95931	16.044188	1892.427	1261.527	11.432153	2.090645
18	0.6322316	46.12607	19.985617	1902.237	1268.066	11.022080	2.091855
19	0.5393913	69.24099	27.226664	1907.320	1271.455	10.398572	2.092033
20	0.4137403	129.98786	41.111349	1904.247	1269.406	9.435012	2.090873
21	0.3489800	176.61948	50.416057	1895.155	1263.345	8.864124	2.088809

	x	xd	R5P	Pi
1	0.03071716	2.314841	18	1400
2	0.03072109	2.314923	18	1400
3	0.03072339	2.314970	18	1400
4	0.03072430	2.314989	18	1400
5	0.03072446	2.314992	18	1400
6	0.03072417	2.314986	18	1400
7	0.03072362	2.314975	18	1400
8	0.03072293	2.314961	18	1400

```
9  0.03072219 2.314945  18 1400
10 0.03072145 2.314930  18 1400
11 0.02764865 2.083423  18 1400
12 0.02797137 2.090083  18 1400
13 0.02864634 2.103833  18 1400
14 0.02932256 2.117375  18 1400
15 0.02981163 2.127028  18 1400
16 0.02997706 2.130268  18 1400
17 0.02969620 2.124760  18 1400
18 0.02888137 2.108565  18 1400
19 0.02756771 2.081744  18 1400
20 0.02615490 2.051844  18 1400
21 0.02585793 2.045410  18 1400
```

Clearly, this system has stability sensitivity problems.

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

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

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

```
> summary(curto)

$nSpecies
[1] 18
```

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

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

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

$nStates
[1] 16

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

$nReactions
[1] 37

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

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

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

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

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

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

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

	[,15]	[,16]	[,17]	[,18]	[,19]	[,20]	[,21]	[,22]	[,23]	[,24]	[,25]	[,26]
PRPP	0	0	0	0	0	-1	0	0	-1	0	0	0
IMP	0	0	1	0	0	0	0	0	1	0	0	-1
SAMP	0	0	0	0	0	0	0	0	0	0	0	0
ATP	0	0	0	0	0	0	0	0	0	0	0	0
SAM	0	0	0	0	0	0	0	0	0	0	0	0
Ade	0	0	0	0	0	0	0	0	0	0	0	0
XMP	0	0	0	-1	0	0	0	0	0	0	0	1
GTP	0	-1	-1	1	-1	1	-1	0	0	0	0	0
dATP	0	0	0	0	0	0	0	0	0	0	0	0
dGTP	-1	1	0	0	0	0	0	0	0	0	0	0
RNA	0	0	0	0	0	0	1	0	0	0	0	0
DNA	1	0	0	0	0	0	0	0	0	0	0	0
HX	0	0	0	0	0	0	0	0	-1	-1	-1	0
Xa	0	0	0	0	0	0	0	1	0	0	1	0
Gua	0	0	0	0	1	-1	0	-1	0	0	0	0
UA	0	0	0	0	0	0	0	0	0	0	0	0

	[,27]	[,28]	[,29]	[,30]	[,31]	[,32]	[,33]	[,34]	[,35]	[,36]	[,37]
PRPP	0	0	0	1	-1	0	0	0	0	0	0
IMP	-1	0	0	0	0	0	0	0	0	0	0
SAMP	0	0	0	0	0	0	0	0	0	0	0
ATP	0	-1	0	0	0	1	0	1	0	0	0
SAM	0	1	-1	0	0	0	0	-1	0	0	0
Ade	0	0	1	0	0	0	0	0	0	0	0
XMP	0	0	0	0	0	0	0	0	0	0	0
GTP	0	0	0	0	0	0	1	0	0	0	0
dATP	0	0	0	0	0	0	0	0	0	0	0
dGTP	0	0	0	0	0	0	0	0	0	0	0
RNA	0	0	0	0	0	-1	-1	0	0	0	0
DNA	0	0	0	0	0	0	0	0	0	0	0
HX	1	0	0	0	0	0	0	0	0	0	0
Xa	0	0	0	0	0	0	0	0	0	-1	-1
Gua	0	0	0	0	0	0	0	0	0	0	0
UA	0	0	0	0	0	0	0	0	-1	0	1

```
$nRules
[1] 0

$ruleIDs
NULL

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

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

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

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

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

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

> curto

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


$id
[1] "curto"

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

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

$compartments$cell$size
[1] 1



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

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

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

$species$PRPP$bc
[1] FALSE


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

$species$IMP$ic
[1] 98.2634

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

$species$IMP$bc
[1] FALSE


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

$species$SAMP$ic
[1] 0.198189

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

$species$SAMP$bc
[1] FALSE


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

$species$ATP$ic
[1] 2475.35

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

$species$ATP$bc
```

```
[1] FALSE


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

$species$SAM$ic
[1] 3.99187

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

$species$SAM$bc
[1] FALSE


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

$species$Ade$ic
[1] 0.98473

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

$species$Ade$bc
[1] FALSE


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

$species$XMP$ic
[1] 24.793

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

$species$XMP$bc
[1] FALSE


$species$GTP
```

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

$species$GTP$ic
[1] 410.223

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

$species$GTP$bc
[1] FALSE


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

$species$dATP$ic
[1] 6.01413

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

$species$dATP$bc
[1] FALSE


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

$species$dGTP$ic
[1] 3.02581

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

$species$dGTP$bc
[1] FALSE


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

$species$RNA$ic
```

```
[1] 28680.5

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

$species$RNA$bc
[1] FALSE


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

$species$DNA$ic
[1] 5179.34

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

$species$DNA$bc
[1] FALSE


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

$species$HX$ic
[1] 9.51785

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

$species$HX$bc
[1] FALSE


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

$species$Xa$ic
[1] 5.05941

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

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


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

$species$Gua$ic
[1] 5.50638

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

$species$Gua$bc
[1] FALSE


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

$species$UA$ic
[1] 100.293

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

$species$UA$bc
[1] FALSE


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

$species$R5P$ic
[1] 18

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

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

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

$species$Pi$ic
[1] 1400

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

$species$Pi$bc
[1] TRUE



$globalParameters
list()

$rules
list()

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

$reactions$ada$reversible
[1] FALSE

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

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

$reactions$ada$parameters
    aada    fada4
0.001062 0.970000

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

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

$reactions$ada$exprLaw
aada * ATP^fada4

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

$reactions$ada$law
function (r, p = NULL)
{
    aada = p["aada"]
    fada4 = p["fada4"]
    ATP = r["ATP"]
    aada * ATP^fada4
}
<environment: 0x239ab38>


$reactions$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: 0x832440>


$reactions$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: 0x1fe86f0>


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

$reactions$adrnr$reversible
[1] FALSE

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

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

$reactions$adrnr$products
[1] "dATP"
```

```
$reactions$adrnr$parameters
  aadrnr  fadrnr4  fadrnr9 fadrnr10
  0.0602   0.1000  -0.3000   0.8700

$reactions$adrnr$mathmlLaw
<apply>
 <times/>
 <apply>
  <times/>
  <apply>
   <times/>
   <ci>aadrnr</ci>
   <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fadrnr4</ci>
   </apply>
  </apply>
  <apply>
   <power/>
   <ci>dATP</ci>
   <ci>fadrnr9</ci>
  </apply>
 </apply>
 <apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fadrnr10</ci>
 </apply>
</apply>

$reactions$adrnr$exprLaw
aadrnr * ATP^fadrnr4 * dATP^fadrnr9 * dGTP^fadrnr10

$reactions$adrnr$strLaw
[1] "aadrnr*ATP^fadrnr4*dATP^fadrnr9*dGTP^fadrnr10"

$reactions$adrnr$law
function (r, p = NULL)
{
    aadrnr = p["aadrnr"]
    fadrnr4 = p["fadrnr4"]
    fadrnr9 = p["fadrnr9"]
    fadrnr10 = p["fadrnr10"]
    ATP = r["ATP"]
    dGTP = r["dGTP"]
```

```
    dATP = r["dATP"]
    aadrnr * ATP^fadrnr4 * dATP^fadrnr9 * dGTP^fadrnr10
}
<environment: 0x2254398>


$reactions$ampd
$reactions$ampd$id
[1] "ampd"

$reactions$ampd$reversible
[1] FALSE

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

$reactions$ampd$modifiers
[1] "GTP" "Pi"

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

$reactions$ampd$parameters
   aampd   fampd4   fampd8  fampd18
 0.02688  0.80000 -0.03000 -0.10000

$reactions$ampd$mathmlLaw
<apply>
 <times/>
 <apply>
  <times/>
  <apply>
   <times/>
   <ci>aampd</ci>
   <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fampd4</ci>
   </apply>
  </apply>
  <apply>
   <power/>
   <ci>GTP</ci>
   <ci>fampd8</ci>
  </apply>
 </apply>
```

```
 <apply>
  <power/>
  <ci>Pi</ci>
  <ci>fampd18</ci>
 </apply>
</apply>

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

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

$reactions$ampd$law
function (r, p = NULL)
{
    aampd = p["aampd"]
    fampd4 = p["fampd4"]
    fampd8 = p["fampd8"]
    fampd18 = p["fampd18"]
    ATP = r["ATP"]
    GTP = r["GTP"]
    Pi = r["Pi"]
    aampd * ATP^fampd4 * GTP^fampd8 * Pi^fampd18
}
<environment: 0x21355e8>


$reactions$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: 0x22cde28>


$reactions$arna
$reactions$arna$id
[1] "arna"

$reactions$arna$reversible
[1] FALSE

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

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

$reactions$arna$products
[1] "RNA"

$reactions$arna$parameters
 aarna frnap4 frnap8
614.50   0.05   0.13

$reactions$arna$mathmlLaw
<apply>
 <times/>
 <apply>
  <times/>
  <ci>aarna</ci>
  <apply>
   <power/>
   <ci>ATP</ci>
   <ci>frnap4</ci>
  </apply>
 </apply>
 <apply>
  <power/>
  <ci>GTP</ci>
  <ci>frnap8</ci>
 </apply>
</apply>

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

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

$reactions$arna$law
function (r, p = NULL)
{
    aarna = p["aarna"]
    frnap4 = p["frnap4"]
    frnap8 = p["frnap8"]
    ATP = r["ATP"]
    GTP = r["GTP"]
    aarna * ATP^frnap4 * GTP^frnap8
}
<environment: 0x2067100>


$reactions$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: 0x22a7cc0>
```

```
$reactions$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: 0x21dbd50>


$reactions$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: 0x1da7440>


$reactions$den
$reactions$den$id
[1] "den"

$reactions$den$reversible
[1] FALSE

$reactions$den$reactants
[1] "PRPP"

$reactions$den$modifiers
[1] "dGTP" "IMP"  "ATP"  "GTP"  "Pi"

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

$reactions$den$parameters
   aden   fden1   fden2   fden4   fden8  fden18
 5.2728  2.0000 -0.0600 -0.2500 -0.2000 -0.0800

$reactions$den$mathmlLaw
<apply>
 <times/>
 <apply>
  <times/>
  <apply>
   <times/>
   <apply>
    <times/>
    <apply>
     <times/>
     <ci>aden</ci>
     <apply>
```

```
      <power/>
      <ci>PRPP</ci>
      <ci>fden1</ci>
     </apply>
    </apply>
    <apply>
     <power/>
     <ci>IMP</ci>
     <ci>fden2</ci>
    </apply>
   </apply>
   <apply>
    <power/>
    <ci>ATP</ci>
    <ci>fden4</ci>
   </apply>
  </apply>
  <apply>
   <power/>
   <ci>GTP</ci>
   <ci>fden8</ci>
  </apply>
 </apply>
 <apply>
  <power/>
  <ci>Pi</ci>
  <ci>fden18</ci>
 </apply>
</apply>

$reactions$den$exprLaw
aden * PRPP^fden1 * IMP^fden2 * ATP^fden4 * GTP^fden8 * Pi^fden18

$reactions$den$strLaw
[1] "aden*PRPP^fden1*IMP^fden2*ATP^fden4*GTP^fden8*Pi^fden18"

$reactions$den$law
function (r, p = NULL)
{
    aden = p["aden"]
    fden1 = p["fden1"]
    fden2 = p["fden2"]
    fden4 = p["fden4"]
    fden8 = p["fden8"]
    fden18 = p["fden18"]
    PRPP = r["PRPP"]
```

```
    dGTP = r["dGTP"]
    IMP = r["IMP"]
    ATP = r["ATP"]
    GTP = r["GTP"]
    Pi = r["Pi"]
    aden * PRPP^fden1 * IMP^fden2 * ATP^fden4 * GTP^fden8 * Pi^fden18
}
<environment: 0x1f97ee8>


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

$reactions$dgnuc$reversible
[1] FALSE

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

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

$reactions$dgnuc$parameters
  adgnuc fdgnuc10
 0.03333  1.00000

$reactions$dgnuc$mathmlLaw
<apply>
 <times/>
 <ci>adgnuc</ci>
 <apply>
  <power/>
  <ci>dGTP</ci>
  <ci>fdgnuc10</ci>
 </apply>
</apply>

$reactions$dgnuc$exprLaw
adgnuc * dGTP^fdgnuc10

$reactions$dgnuc$strLaw
[1] "adgnuc*dGTP^fdgnuc10"

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

```
{
    adgnuc = p["adgnuc"]
    fdgnuc10 = p["fdgnuc10"]
    dGTP = r["dGTP"]
    adgnuc * dGTP^fdgnuc10
}
<environment: 0x1e38e20>


$reactions$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: 0x1f9d2d8>


$reactions$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: 0x1db1250>


$reactions$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: 0x1b19638>


$reactions$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: 0x2255838>


$reactions$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: 0x1b9a200>


$reactions$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: 0x1d87c10>


$reactions$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: 0x2062638>


$reactions$gprt
$reactions$gprt$id
[1] "gprt"

$reactions$gprt$reversible
[1] FALSE

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

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

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

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

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

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

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

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

$reactions$gprt$law
function (r, p = NULL)
{
    agprt = p["agprt"]
    fgprt1 = p["fgprt1"]
    fgprt8 = p["fgprt8"]
    fgprt15 = p["fgprt15"]
    Gua = r["Gua"]
    PRPP = r["PRPP"]
    GTP = r["GTP"]
    agprt * PRPP^fgprt1 * GTP^fgprt8 * Gua^fgprt15
}
<environment: 0x22ccb48>


$reactions$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: 0x218d080>


$reactions$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: 0x1309768>


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

$reactions$hprt$reversible
[1] FALSE

$reactions$hprt$reactants
```

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

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

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

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

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

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

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

$reactions$hprt$law
```

```
function (r, p = NULL)
{
    ahprt = p["ahprt"]
    fhprt1 = p["fhprt1"]
    fhprt2 = p["fhprt2"]
    fhprt13 = p["fhprt13"]
    HX = r["HX"]
    PRPP = r["PRPP"]
    IMP = r["IMP"]
    ahprt * PRPP^fhprt1 * IMP^fhprt2 * HX^fhprt13
}
<environment: 0x22f7548>


$reactions$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: 0x1e86f38>


$reactions$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: 0x143f900>


$reactions$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: 0x232a4c8>


$reactions$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: 0x2065c08>


$reactions$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: 0x13d7c30>


$reactions$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: 0x233c238>


$reactions$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: 0x21b4210>


$reactions$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: 0x1015590>
```

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

$reactions$rnaa$reversible
[1] FALSE

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

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

$reactions$rnaa$parameters
  arnaa frnan11
0.06923 1.00000

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

$reactions$rnaa$exprLaw
arnaa * RNA^frnan11

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

$reactions$rnaa$law
function (r, p = NULL)
{
    arnaa = p["arnaa"]
    frnan11 = p["frnan11"]
    RNA = r["RNA"]
    arnaa * RNA^frnan11
}
<environment: 0x22ffa58>
```

```
$reactions$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: 0x1edfda8>
```

```
$reactions$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: 0x16c9b50>


$reactions$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: 0x2296c68>


$reactions$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: 0x2190f08>


$reactions$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: 0x131eb68>



$htmlNotes
<notes>
 <body xmlns="http://www.w3.org/1999/xhtml">
  <p>This is a purine metabolism model that is geared toward studies of gout.</p>
  <p>The model is fully described in Curto et al., MBSC 151 (1998) pp 1-49</p>
  <p>The model uses Generalized Mass Action (GMA;i.e. power law) descriptions of reaction ra
  <p>Such descriptions are local approximations that assume independent substrate binding.</
  <p/>
  <p>The de novo purine flux vden= 2.39 is in umole/min/KG, i.e. 2.4*60=144 uM/h if we let e
```

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

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