

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 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	

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 bumps
```

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

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

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

```

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

```

Clearly, this system has stability sensitivity problems.

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

```

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

```

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

```
> summary(curto)
```

```
$nSpecies
[1] 18
```

\$sIDs

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

\$S0

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

\$BC

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

\$nStates

```
[1] 16
```

\$y0

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

\$nReactions

```
[1] 37
```

\$rIDs

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

\$rLaws

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

"aadna*dATP^fdnap9*dGTP^fdnap10"
 adnr
 "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"
 gmpr
 "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	hprt	hx
	4.807078e+00	3.738009e+00	1.323532e+03	1.154277e+00	3.669760e+00	4.730928e-02
	hxd	impd	inuc	mat	polyam	prpps
	1.191281e+00	1.595762e+00	2.642505e+00	1.498849e+01	1.007991e+00	2.088492e+01
	pyr	rnaa	rnag	trans	ua	x
	9.999890e+00	1.985551e+03	1.323605e+03	1.398050e+01	2.314825e+00	3.071716e-02
	xd					
	2.314841e+00					

\$globalVec

NULL

\$incid

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

IMP	0	0	0	0	1	0	0	-1	0	0	1	0	0	0
SAMP	0	0	0	0	0	0	0	1	-1	0	0	0	0	0
ATP	-1	0	0	-1	-1	1	-1	0	1	0	0	0	0	0
SAM	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ade	0	-1	0	0	0	-1	0	0	0	0	0	0	0	0
XMP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GTP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
dATP	0	0	-1	1	0	0	0	0	0	-1	0	0	1	0
dGTP	0	0	0	0	0	0	0	0	0	0	0	-1	0	1
RNA	0	0	0	0	0	0	1	0	0	0	0	0	0	0
DNA	0	0	1	0	0	0	0	0	0	0	0	0	-1	-1
HX	1	0	0	0	0	0	0	0	0	1	0	0	0	0
Xa	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Gua	0	0	0	0	0	0	0	0	0	0	0	1	0	0
UA	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	[,15]	[,16]	[,17]	[,18]	[,19]	[,20]	[,21]	[,22]	[,23]	[,24]	[,25]	[,26]		
PRPP	0	0	0	0	0	-1	0	0	-1	0	0	0	0	0
IMP	0	0	1	0	0	0	0	0	1	0	0	0	-1	0
SAMP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ATP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SAM	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ade	0	0	0	0	0	0	0	0	0	0	0	0	0	0
XMP	0	0	0	-1	0	0	0	0	0	0	0	0	1	0
GTP	0	-1	-1	1	-1	1	-1	0	0	0	0	0	0	0
dATP	0	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	0
RNA	0	0	0	0	0	0	1	0	0	0	0	0	0	0
DNA	1	0	0	0	0	0	0	0	0	0	0	0	0	0
HX	0	0	0	0	0	0	0	0	-1	-1	-1	0	0	0
Xa	0	0	0	0	0	0	0	1	0	0	1	0	0	0
Gua	0	0	0	0	1	-1	0	-1	0	0	0	0	0	0
UA	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	[,27]	[,28]	[,29]	[,30]	[,31]	[,32]	[,33]	[,34]	[,35]	[,36]	[,37]			
PRPP	0	0	0	1	-1	0	0	0	0	0	0	0	0	0
IMP	-1	0	0	0	0	0	0	0	0	0	0	0	0	0
SAMP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ATP	0	-1	0	0	0	1	0	1	0	0	0	0	0	0
SAM	0	1	-1	0	0	0	0	-1	0	0	0	0	0	0
Ade	0	0	1	0	0	0	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	1	0	0	0	0	0	0	0
dATP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
dGTP	0	0	0	0	0	0	0	0	0	0	0	0	0	0
RNA	0	0	0	0	0	-1	-1	0	0	0	0	0	0	0
DNA	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HX	1	0	0	0	0	0	0	0	0	0	0	0	0	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
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*GTP^fampd8*Pi^fampd18
aprr	aaprr*PRPP^faprr1*ATP^faprr4*Ade^faprr6
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}
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	
gprr	3.738009e+00	
grna	1.323532e+03	
gua	1.154277e+00	
hprt	3.669760e+00	
hx	4.730928e-02	
hxd	1.191281e+00	
impd	1.595762e+00	
inuc	2.642505e+00	
mat	1.498849e+01	
polyam	1.007991e+00	

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

```
> curto
```

```
$sbml
```

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

```
$id
```

```
[1] "curto"
```

```
$notes
```

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

```
$compartments
```

```
$compartments$cell
```

```
$compartments$cell$id
```

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

```
$compartments$cell$size
```

```
[1] 1
```

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

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

```
$species
```

```
$species$PRPP
```

\$species\$PRPP\$id

[1] "PRPP"

\$species\$PRPP\$ic

[1] 5

\$species\$PRPP\$compartment

[1] "cell"

\$species\$PRPP\$bc

[1] FALSE

\$species\$IMP

\$species\$IMP\$id

[1] "IMP"

\$species\$IMP\$ic

[1] 98.2634

\$species\$IMP\$compartment

[1] "cell"

\$species\$IMP\$bc

[1] FALSE

\$species\$SAMP

\$species\$SAMP\$id

[1] "SAMP"

\$species\$SAMP\$ic

[1] 0.198189

\$species\$SAMP\$compartment

[1] "cell"

\$species\$SAMP\$bc

[1] FALSE

\$species\$ATP

\$species\$ATP\$id

[1] "ATP"

\$species\$ATP\$ic

[1] 2475.35

\$species\$ATP\$compartment

[1] "cell"

\$species\$ATP\$bc

[1] FALSE

\$species\$SAM

\$species\$SAM\$id

[1] "SAM"

\$species\$SAM\$ic

[1] 3.99187

\$species\$SAM\$compartment

[1] "cell"

\$species\$SAM\$bc

[1] FALSE

\$species\$Ade

\$species\$Ade\$id

[1] "Ade"

\$species\$Ade\$ic

[1] 0.98473

\$species\$Ade\$compartment

[1] "cell"

\$species\$Ade\$bc

[1] FALSE

\$species\$XMP

\$species\$XMP\$id

[1] "XMP"

\$species\$XMP\$ic

[1] 24.793

\$species\$XMP\$compartment

[1] "cell"

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

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

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

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

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

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

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

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

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

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

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

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

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

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

```
$species$RNA$ic
[1] 28680.5
```

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

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

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

```
$species$DNA$ic
[1] 5179.34
```

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

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

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

```
$species$HX$ic
[1] 9.51785
```

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

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

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

\$species\$Xa\$ic

[1] 5.05941

\$species\$Xa\$compartment

[1] "cell"

\$species\$Xa\$bc

[1] FALSE

\$species\$Gua

\$species\$Gua\$id

[1] "Gua"

\$species\$Gua\$ic

[1] 5.50638

\$species\$Gua\$compartment

[1] "cell"

\$species\$Gua\$bc

[1] FALSE

\$species\$UA

\$species\$UA\$id

[1] "UA"

\$species\$UA\$ic

[1] 100.293

\$species\$UA\$compartment

[1] "cell"

\$species\$UA\$bc

[1] FALSE

\$species\$R5P

\$species\$R5P\$id

[1] "R5P"

\$species\$R5P\$ic

[1] 18

```
$species$R5P$compartment
```

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

```
$species$R5P$bc
```

```
[1] TRUE
```

```
$species$Pi
```

```
$species$Pi$id
```

```
[1] "Pi"
```

```
$species$Pi$ic
```

```
[1] 1400
```

```
$species$Pi$compartment
```

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

```
$species$Pi$bc
```

```
[1] TRUE
```

```
$globalParameters
```

```
list()
```

```
$rules
```

```
list()
```

```
$reactions
```

```
$reactions$ada
```

```
$reactions$ada$id
```

```
[1] "ada"
```

```
$reactions$ada$reversible
```

```
[1] FALSE
```

```
$reactions$ada$reactants
```

```
[1] "ATP"
```

```
$reactions$ada$products
```

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

```
$reactions$ada$parameters
```

```
  aada  fada4
```

```
0.001062 0.970000
```



```

$reactions$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: 0x229f7d0>

```

```

$reactions$aade
$reactions$aade$id
[1] "ade"

```

```

$reactions$aade$reversible
[1] FALSE

```

```

$reactions$aade$reactants
[1] "Ade"

```

```

$reactions$aade$parameters
aade fade6
0.01 0.55

```

```

$reactions$aade$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: 0x178be78>

$reactions$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: 0x2e96a38>

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

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

$reactions$adnrn$strLaw
[1] "adnrn*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: 0x2f03a38>

```

```

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

```

```

$reactions$aampd$reversible
[1] FALSE

```

```

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

```

```

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

```

```

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

```

```

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

```

```

$reactions$aampd$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: 0x2fa1308>

```

```

$reactions$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>
  <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: 0x3021d70>

```

```

$reactions$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
  arna 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>

$reactions$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: 0x30d99f8>

$reactions$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>
    <power/>
    <ci>GTP</ci>
    <ci>fasuc8</ci>
  </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: 0x315ee78>

```

```

$reactions$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: 0x31ecf38>

```

```

$reactions$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: 0x3231308>

$reactions$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: 0x32d69d0>

```

```

$reactions$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: 0x33aa488>

$reactions$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: 0x3378e28>

$reactions$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: 0x3346ca0>
```

```
$reactions$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: 0x3307e70>

$reactions$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: 0x32a79f8>

```

```

$reactions$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: 0x31fe0a8>

```

```

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

```

```

$reactions$gmpr$gmps$reversible
[1] FALSE

```

```

$reactions$gmpr$gmps$reactants
[1] "XMP"

```

```

$reactions$gmpr$gmps$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: 0x3175828>

$reactions$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: 0x3119b00>

```

```

$reactions$gpprt
$reactions$gpprt$id
[1] "gpprt"

```

```

$reactions$gpprt$reversible
[1] FALSE

```

```

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

```

```

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

```

```

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

```

```

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

```

```

$reactions$gpprt$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: 0x308c2c0>

$reactions$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: 0x2fe1f58>

$reactions$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: 0x2f93308>

$reactions$hpert
$reactions$hpert$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

$reactions$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: 0x2f03e78>

```

```

$reactions$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: 0x2eb1dd0>

$reactions$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: 0x2e77300>

$reactions$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: 0x29a23a0>

```

```

$reactions$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: 0x239ff60>

\$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: 0x209fd68>
```

```
$reactions$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: 0x1c806e8>
```

```
$reactions$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: 0x33e73b8>

$reactions$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: 0x342bc68>

```

```

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

$reactions$rnaa$reversible
[1] FALSE

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

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

$reactions$rnaa$parameters
  arnaa frnan11
0.06923 1.00000

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

$reactions$rnaa$exprLaw
arna * RNA^frnan11

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

$reactions$rnaa$law
function (r, p = NULL)
{
  arna = p["arna"]

```



```

    frnan11 = p["frnan11"]
    RNA = r["RNA"]
    arnaa * RNA^frnan11
}
<environment: 0x34597d8>

```

```

$reactions$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: 0x3488390>

```

```

$reactions$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: 0x34b5f70>

$reactions$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: 0x34e4a48>

```

```

$reactions$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: 0x35125b8>

$reactions$x$d
$reactions$x$d$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: 0x3541100>
```

```
$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"
```