SUPPLEMENTARY RESULTS

A package and a workspace to personalize and trace GSM reconstruction

Adaptability to various input data and databases. The PADMet package enables users to link admissible input data to the customized workflows and the various analysis tools available in the workspace (Fig. 1). The *AuReMe* workspace is encapsulated in a Docker image with a "toy" dataset along with versions of MetaCyc 20.0, MetaCyc 20.5 and BiGG 2.3 databases. The purpose of the Docker encapsulation is to provide a workspace that can easily be used with the most diverse set of operating systems (Linux, MacOS, Windows). *PADMet* format ensures the interoperability of knowledge, tools and data. Accepted inputs are genome Genbank files (gbk or gbff), protein sequence fasta files (faa), metabolic models Systems Biology Markup Language files (SBML (1)) for studied or template organisms, Pathway/Genome Databases (PGDB) resulting from Pathway Tools workflows and text files for gene expression data, growth media composition, metabolic targets or biomass components (Fig. 1). An individual can also input a whole new database of reactions and metabolites in a tab-separated value format.

Customization of a pre-set pipeline. The *AuReMe* workspace enables the merging of multiple draft models for an organism under study. Fig. 3 depicts several customizations of pipelines as well as the pre-set pipeline available in the workspace. The latter will import the results of an annotation-based reconstruction of Pathway Tools (PathoLogic) (2) and run a single-template orthology-based reconstruction with Pantograph (3) which reports a consensus between both OrthoMCL (4) and Inparanoid (5). Both models are merged with the *PADmet* package prior performing functional analysis. The functional analysis of a reconstructed metabolic network can be performed at the graph-based level with MeneTools (see Methods) or at the stoichiometric-based level with the functionalities of the pre-installed CobraPy (6) and Psamm (7) packages. When required, reactions can be suggested to fill the network and enable functionality of the GSM. Several tools can be exploited, either separately or iteratively. Meneco, a graph-based gap-filling technique (8) allows the topology of the network to be completed; which can be useful when dealing with exotic organisms. The GapFill (9) or the fastGapFill algorithm (10) allow flux-based completions of the model. The last two are implemented in the pre-installed Psamm (7) package.

Wiki-based exploration of metabolic networks: a novel method to explore and monitor GSM reconstructions and their associated metadata.

GSM information can be displayed in the wiki according to its origin: orthology, genome annotation, gapfilling or manual curation.

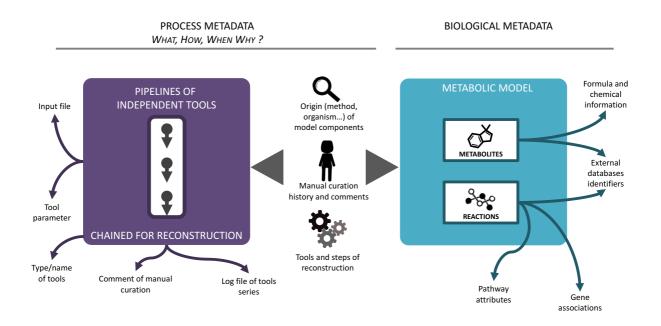
Wikis powered by AuReMe display the two families of metadata described in the article. Biological metadata supported by wikis encompass i) all initial data related to an imported model (e.g. conservation of original stoichiometry of reactions, gene associations, data from the 'note' section of SBML model files, etc.), ii) the reasons that led to a curation of the model, i.e., why a reaction/metabolite was added or deleted (this information is stored when the user completes a form to curate the model), iii) the

corresponding identifiers from different databases for most of the reactions and compounds and iv) the traceability of compounds used as seeds (e.g. growth medium compounds) and targets (compounds known to be produced or biomass components) during model simulations (Supp. Fig. A). GSM reconstruction process metadata include i) the source of each reaction and compound (output of a tool/reconstruction step or organism origin of the model for multispecies modeling), ii) the version of the metabolic database used for data standardization, iii) the steps and tools used during the reconstruction process and iv) the manual curation history i.e. all the *a posteriori* modifications made to the model (Supp. Fig. A).

Wiki pages related to genes, reactions, metabolites or pathways contain both static and linked information. Names, synonyms, formulas, etc., are displayed, in accordance with the data of the original reference database (MetaCyc, BiGG) used to reconstruct the GSM. Links to the latter or other databases (UniProt, Orcae, KEGG) enable the user to easily find external additional information about a gene, a protein or another component of the GSM.

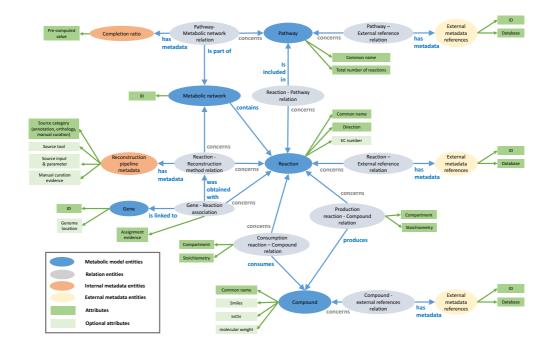
SUPPLEMENTARY FIGURES

Supplementary Figure A. Description of metadata associated to the model or its reconstruction and managed by the AuReMe workspace for storage and wiki-visualization. Biological metadata are related to reactions and metabolites, as well as external identifiers to connect information to other databases. Process metadata describes the history of the modifications applied to the model: steps of reconstruction, manual curation history and origin of model components (which tool, at which step, with which parameter or input file, etc.). Process metadata connect the model with the series of tools that was used to produce it.



Supplementary Figure B. Abstraction of the RDF semantic-based graph used to represent metabolic models. RDF schema provides data-modeling vocabulary for RDF data. The entities are

linked by relations and may have specific properties (attributes). Some entities used are a cornerstone between two entities to enrich the relation (relation entities). The external metadata entities allow compounds, reactions and pathways to link to external databases such as MetaCyc, BiGG, UniProt and KEGG. The internal metadada entities allow reactions, gene, pathways and metabolic networks to link to information relative either to reconstruction pipeline information or to metabolic network characteristics.



SUPPLEMENTARY TABLE

Supplementary Table A. Impact of the various pipeline steps on the functionality of the built GSM. Network column describes the methodology used at each step of the pipeline. The functionality of each intermediary network was test according to the production of biomass (FBA growth rate), and more generally to the production of a predetermined family of compounds of interest (targets), which contain all the biomass components, with respect to each species.

Organism GSM	Subnetworks of the reconstruction pipeline	number of metabolites	number of reactions	number of genes	ratio of reactions associated to genes	Number of biological compounds of interest (targets)	number of topologically producible targets	number of flux activated targets	FBA growth rate
	annotation-based network	2118	1834	2281	83%		5	5	0
	orthology with A. thaliana	650	442	593	89%		1	0	0
E. siliculosus	merging annotation and orthology-based models	2118	1887	2281	83%	50	5	5	0
	Final network after gap-filling and manual curation	2132	1977	2281	79%		50	50	3,02
	orthology with E. coli str. K-12 substr. MG1655	728	715	470	100%		4	27	0
	orthology with L. plantarum WCFS1	472	400	398	100%		4	27	0
Enterococcus faecalis str. v583	orthology with B. subtilis subsp. subtilis str. 168	506	465	374	100%	92	9	27	0
	merging orthology-based models	937	1192	669	92%		13	37	0
	Final network after gap-filling and manual curation	911	1117	613	84%		72	92	22,54
	experimental annotations	1108	872	482	75%		0	0	0
	in silico annotations	2088	1696	1855	80%	38	0	0	0
	orthology with A. thaliana	621	366	408	100%		0	0	0
	orthology with C. reinhardtii	497	503	408	100%		0	0	0
T. lutea	orthology with E. siliculosus	1590	1139	1163	100%		0	0	0
	orthology with Synechocystis sp. PCC 6803	353	207	275	100%		0	0	0
	primary network	285	208	0	0%		0	0	0
	merged models	2743	2779	2728	88%		5	38	74,54
	Final network after gap-filling and manual curation	2749	2796	2728	87%		19	38	74,54
	orthology with Clostridium iHN637	492	352	297	100%		4	3	0
	orthology with B. subtilis iYO844	601	507	400	100%		7	3	0
S. thermosulfidooxidans str. Cutipay	orthology with A. ferroaxidans iMCS07	450	309	288	100%	66	4	3	0
-	merging annotation and orthology-based models	831	949	574	91%		23	3	0
	Final network after manual curation	854	1067	541	69%		62	66	6,4

SUPPLEMENTARY METHODS

AuReMe environment user interface and customizability

For all reconstructed networks, The GSM reconstruction workflow was described in a configuration file (called Makefile), which handled the reconstruction process by running simple commands such as: make orthology-based, make annotation-based, make draft, and make gapfilling. The last two commands run the first two provided they had not been run yet and the corresponding data are available. The configuration file could be personalized in order to select the tools used for each step of the reconstruction workflow. The network analysis was handled through the commands make curation, make menecheck, and make fbacheck. The creation of the wiki pages was handled by make wikipage.

Local and webserver wiki creation

The creation of the wiki for *E. siliculosus* (http://gem-aureme.irisa.fr/ectogem) and *T. lutea* (http://gemaureme.irisa.fr/tisogem) GSMs was handled in two steps. First, the commands make wikipages in the *AuReMe* workspace launched the creation of the wiki pages for genes, metabolites, pathways and reactions in a local repository of the workspace. Second, the commands make build and make send-allpages launched the creation of a preconfigured Docker container hosting the wiki infrastructure which could be locally accessed through a web-interface. This local wiki was used to perform the manual exploration and curation of the metabolic reconstructions. Once the networks were curated, the command make web-send-pages uploaded the wiki pages to the webserver on which the Mediawiki technology had been previously installed.

Turning metabolic network information into a RDF triplestore

The script padmet-to-tsv from the module connection of padmet-utils was used to export relations between the entities of the *T. lutea* model that we obtain and the MetaCyc database in padmet format

as TSV files. Based on the RDF graph, shown in Supp. Fig. B, these files were transcribed into RDF triple which were stored into a SPARQL endpoint freely accessible at http://bit.ly/tisoSparql. This representation performed various complicated and precise queries and also made the junction to other databases such as MetaCyc, BiGG, KEGG and UniProt. Based on the latter, SPARQL requests were generated to exhibit pathways which contain exclusive reactions from different sources.

The PADMet library and PADMet-utils

The *PADMet*-utils is a suite of scripts based on *PADMet* library to link admissible input data to the customized workflows and the various analysis tools available in the workspace. The *PADMet*-utils Is contains four main modules for data management, connection to software, data exploration and manual curation assistance. For instance, pgdb-to-padmet from the module connection to software was used to compile the output of Pathway Tools, the PGDB folder to one unique file in *PADMet* format. In the same module, sbml-to-padmet was used to convert one or more SBML to one unique file in *PADMet* format with or without a database of reference. add-seeds-rxn from the module data management was used to add the exchange and transport reactions of a set of metabolites in a given metabolic network. fba-test from the module data exploration was used to perform FBA. To get an idea of the way to use the *PADMet*-utils simply explore the Makefile of *AuReMe*. This toolbox only requires the *PADMet* library and is available in the *AuReMe* workspace or can be downloaded on Gitlab https://gitlab.inria.fr/maite/padmet-utils and used in stand-alone mode.

Exporting a model produced in the workspace to Pathway Tools

AuReMe can be used as an intermediary between the creation of of model in a major platform such as Pathway Tools and its further publication. This enables individual tools to be applied to the model to modify or enhance it while monitoring and tracing the processes. *AuReMe* provides exports in several formats, including a SBML that includes the new reactions and that can be imported into Pathway Tools to re-create a PGDB that can later be published with BioCyc.

The reconstruction of *Ectocarpus siliculosus* metabolic network carried out using the *AuReMe* workflow was built using an initial annotation-based reconstruction made on Pathway Tools (ectov2.2cyc 1.0 in esiliculosus_PGDBs available on http://aureme.genouest.org/suppdata.html), a template model for orthology-based reconstruction (from *Arabidopsis thaliana*) and manual curation.

To go back to the PathwayTools framework we exported the set of reactions added in *AuReMe* in an SBML file and we merged them with the original *Ectocarpus siliculosus* PGDB (ectov2.2cyc), thus creating a new PGDB with the improvements made in *AuReMe*.

To do this, we carried out the following steps:

1) In AureMe, we exported an SBML file with the added reactions:

- Padmet-utils script: sbmlGenerator.py
- output file: added_AureMe_PadMet.xml

Artificial reactions added in *AureMe* for FBA purposes (*i. e.*, exchange reactions) were left out as these reactions are usually not included in PGDBs.

2) In Pathway Tools v 21.0 a new PGDB (addedcyc) was created from the SBML file with added reactions (added_AureMe_PadMet.xml). To do this, in the PathwayTools Pathway/Genome Navigator interface (GUI) we performed the following steps:

Step 1: In the File menu, we selected the option "Import -> SBML File ... ": • File Overviews Pathway Reaction Protein RNA Gene Compound Chromosome SmartTables Tools Help Available Databases Ctrl+H G1655 - Home Back Forward History Next Answer Clone Save DF Summarize Current Database Pathway Tools -- Available Databases Add DB(s) to Available DBs Save Current DB Ctrl+S Save Current DB with Comment Shift+Ctrl+S Pathways Genes (ORF %) Genome Size (bp) Citations C Save PGDB as List Unsaved Changes in Current DB = JCM 1222 = DSM 20088 Revert Current DB. Checkpoint Current DB Updates to File 144 18434 (35.6%) 196.804.589 1351 343 4657 (17.4%) 4,641,652 33232 Restore Updates from Checkpoint File... 2526 11639 (0.6%) 0 52840 Refresh All Open DBs Create New Version for Selected DBs Copyright Notice Configure New DB from MySQL Delete a DB... Attempt to Reconnect to Database Server Save Display State to File Restore Display State from File Print Ctrl+P Frames from Spreadsheet-Format File. Import ▷ Frames from Lisp-Format File. Export DB Links from File... Create Citations from PubMed Exit Ctrl+Q Protein Features from UniProt Phenotype Microarray Data from Spreadsheet or OPM. Quick Search Taxa in the NCBI Taxonomy DB SBML File.. Clear Entire DB from a tar file Test PGDB from File in Drop Box. Import an SBML file into a newly created DB. PGDBs from the Registry

• <u>Step 2</u>: In the SBML import window, we selected the "Create a New Database..." option:

000	X SBML Import
Database Import	
Select an Existing Database	
Create a New Database	
Save DB	
Revert DB	
Exit	
Vorkflow Progress: Read SBML Create compartments Create species and reactions Merge compounds Merge reactions	

• **Step 3:** In the pop-out window we entered the required information to create our new PGDB (addedcyc):

• • •	X Enter Information for New SBML Database
Database (required)	
Organism/Project ID: ADDED Example: ECO	
Version:	Example: 1.0
Database Name: AddedCyc	Example: EcoCyc
DB Storage Type: File 📼	
Taxonomy (required)	
Check box if this is a multi-organism database:	
Organism taxonomic class: 2878	Select the NCBI taxonomy class for this organism. If no taxon currently exists for this organism in the NCBI Taxonomy, or in Metacyc, please Select the most specific (lowest in the taxonomy) possible parent taxon for this organism (preferably a genus or species.) If no appropriate parent taxon exists, please select the closest "unclassified" class. Examples: Escherichia coli K-12 or 83333.
	not find your organism in NCBI Taxonomy or in MetaCyc you need to create a new taxon for it. in such a case select yes and that you selected the correct parent taxon above
Full Species Name: Ectocarpaceae Abbreviated Species Name: E.	
Genome Source:	This information will be appended to the organism name if needed to distinguish this genome from other sequenced genomes for the same organism. We suggest entering the name of the laboratory or institution that performed the sequencing.
NCBI taxonomy ID: 2878 Rank: other	
Phylogenetic Classification: cellular organisms -> E Ectocarpaceae	"karyota -> Stramenopiles -> PX clade -> Phaeophyceae -> Ectocarpales ->
Default Codon Table:	1 Standard 🔲
Mitochondrial Codon Table:	1 Standard 😐
Credits (optional)	
Authors:	Institutions:
OK	

• <u>Step 4</u>: Back in the *SBML import window* we selected the "*Import->Select and Read SBML File …*" command and selected our SBML file with the AureMe

added reactions.

Database	Twport					
. g		ad SBML File				
		Aremene napping				
		pecies (= Compounds) and Reactions ting ecies (= Compounds) pgdbs/user/addedcyc/1.0/data/				
		a land / made a / made a / man / a dida dama / 1 / 0 / data /				
tatus: Initia	Merge SBML Re	actions				
		;; ensure-directories-exist: creating				
to: A log of all most	sages that appear in the	;; /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/reports/ ;; Directory				
nsole window can b	be found in	;; /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/reports/ does				
Users/moortes/SBML-Import-Console-Log-20 7-11-29.txt		;; not exist, will create.				
		;; ensure-directories-exist: creating ;; /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/				
		;; Directory /Dsers/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/				
Workflow Pro	ouress:	;; does not exist, will create.				
	- <u>j</u>	Created addedcvc directory tree.				
Read SBML		Saved /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/input/organism.dat				
Create comp	oartments ies and reactions	Saved /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/input/organism-init.dat				
Merge comp		Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE]				
Merge reacti		[Completed initialization of new PGDB for ADDED]				
		[Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot				
		0 frames ignored				
		9564 frames saved]				
		Saving KB FGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel				
		0 frames ignored				
		3 frames saved]				
		After new changes have been made to the database,				
		they can be saved by the command "Save DB".				
		Alternatively, the command "Revert DB" will undo the changes by				
		resetting the database to the previously saved contents.				
		The next suggested step is to run the command "Import->Select and Read SBML File"				
		SBML Import				
Database	Import	SBML Import				
Database	Import	Saved /osers/mcortes/ploors-rocal/pgdbs/user/addedcyc/i.v/input/organism-init.dat				
Database Prganism:	_	Saved /Users/mcortes/ptools-local/pgdbs/user/addedcyc/l.U/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE.				
Database	_	Saved /0sers/mcortes/ptoors-rocal/pgdbs/user/addedcyc/i.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE]				
Database Prganism: PRG-ID: ADD	_	Saved /Users/mcortes/ptools-local/pqdbs/user/addedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba				
Database organism: oRG-ID: ADD Name: *E.	DED	Saved /Users/mcortes/ptools-local/pgdbs/user/addedcyc/l.U/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot				
Database Prganism: PRG-ID: ADD	DED	Saved /osers/mcortes/ptools-local/pgdbs/user/addedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new FGDE for ADDED] [Saving KE ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored				
Database organism: oRG-ID: ADD Name: *E.	DED	Saved /USEFS/mcortes/ptools-local/pgubs/user/addeddyc/l.v/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addeddyc/1.0/kb/addedbase e.ocelot 0 frames ignored 3564 frames saved]				
Database vrganism: RG-ID: ADD Name: *E. tatus: Modif	DED fied	<pre>Saved /USErS/mcortes/ptools-local/pgdbs/user/sadeadyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel t</pre>				
Database brganism: brG-ID: ADD Name: *E. tatus: Modif bte: A log of all mess oble window can b	DED fied sages that appear in the pe found in	Saved /Users/mcortes/ptools-local/pgdbs/user/addedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3564 frames saved] [Saving KB FGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel. t 0 frames ignored				
Database brganism: brG-ID: ADD Name: *E. tatus: Modif bte: A log of all mess oble window can b	DED fied	<pre>Saved /USErS/mcortes/ptools-local/pgdbs/user/sadeadyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel t</pre>				
Database organism: RG-ID: ADD Name: *E. tatus: Modif ote: A log of all mess nsole window can b ers/morter/SBML	DED fied sages that appear in the pe found in	Saved /USETS/mcOTLES/pLOOIS-IOCAL/pGDS/USET/Addedcyc/1.0/Input/organism-Init.dat Copying class Organisms from METARASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /USETS/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3654 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel 0 frames ignored 36frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel 0 frames ignored 3 frames saved] After new changes have been made to the database,				
Database organism: RG-ID: ADD Name: *E. tatus: Modif ote: A log of all mess nsole window can b ers/morter/SBML	DED fied sages that appear in the pe found in	<pre>Saved /USEFS/mcortes/ploofs-focal/pgubs/user/sadeadyc/1.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB FGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] [After new changes have been made to the database, they can be saved by the command "Save DB".</pre>				
Database organism: RG-ID: ADD Name: *E. tatus: Modif ote: A log of all mess nsole window can b ers/morter/SBML	DED fied sages that appear in the se found in L-Import-Console-Log-20	Saved /USETS/mcOTLES/pLOOIS-IOCAL/pGDS/USET/Addedcyc/1.0/Input/organism-Init.dat Copying class Organisms from METARASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /USETS/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3654 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel 0 frames ignored 36frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel 0 frames ignored 3 frames saved] After new changes have been made to the database,				
Database organism: RG-ID: ADD Name: "E. tatus: Modif tatus: Modif te: A log of all mess noole window can b seramcortes/SBML -11-29.bt Workflow Pro	DED fied sages that appear in the se found in -hmport-Console-Log-20 ogress:	Saved /USEFS/mcortes/ptools-local/pgdbs/user/addeddyc/l.U/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents.				
Database organism: RG-ID: ADD Name: *E. tatus: Modifi- tatus: Modifi- ta	DED fied sages that appear in the pe found in -Import-Console-Log-20 ogress:	<pre>Saved /USEFS/mcortes/ptools-local/pgdbs/user/addedcyc/l.U/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/l.O/kb/addedba e.ocelot 0 frames ignored 3564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel. t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess noole window can b seramcortex/SBML -11-29.txt Workflow Pro Read SBML Create comp	DED fied sages that appear in the ze found in -Import-Console-Log-20 ogress: wartments	<pre>Saved /USEFS/mcortes/ploofs-focal/pgubs/user/sddeddyc/1.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KE ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KE PGDE-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File"</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocrete:XBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /USETS/mcortes/ptools-local/pgubs/user/addedcyc/1.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copyled class hierarchy into ADDEDBASE] [completed initialization of new FGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB FGDE-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SBML File" Command: Select and Read SBML File Reading SBML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif tatus: Modif t	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	Saved /USETS/mcOTLES/pLOOIS-IOCAL/PGDS/USET/Addedcyc/1.0/Input/Organism-Init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /USETS/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3654 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel 0 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /UserSymcortes/ptools-local/pgdbs/user/addedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copyled class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SBML File" Command: Select and Read SEML File Reading SBML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /UserSymcOrtes/ptools=local/pgdbs/user/addedcyc/1.0/input/organism=init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools=local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools=local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import=>Select and Read SEML File" Command: Select and Read SEML File Reading SBML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low=level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /UserS/mcOrtes/ptools-local/pdDS/user/addedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new FGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedbare o.coelot 0 frames ignored 3654 frames saved] [Saving KB FGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocelot t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SBML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /UserS/mcOrtes/ptools-local/pgdbs/user/addedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3654 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel 0 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CCO</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /05er5/mcortes/ptools-local/pgubs/user/addeudyc/1.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KE ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3564 frames saved] [Saving KE PGDE-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDE-METADATA.ocel t 0 frames ignored 3564 frames saved] [After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Dsers/mcortes/Desktop/added_AureMe_PadMet.xml Number of (Low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CC0</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /0sers/mcortes/ptools-local/pgdbs/user/addedcyc/l.0/lnput/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CCO c cytosol cytosol e extracellular extracellular space</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /OSerS/mcortes/ptools-local/pgubs/user/sddedcyc/l.0/input/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/l.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB FGDE-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDE-METADATA.ocel- t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DE". Alternatively, the command "Revert DE" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CCO c cytosol cytosol e extracellular extracellular space After the SEML file was read, the Importer tried to map the compartments</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /OSerS/mcOrtes/ptools-local/pgubs/user/sddedcyc/l.0/input/organism-init.dat Copying class hierarchy into ADDEDBASE] [Completed initialization of new FGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB FGDE-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CCO e cytosol cytosol e extracellular extracellular space After the SEML file was read, the Importer tried to map the compartments described in SEML to the corresponding compartments in the BioCyc ontology. If this mapping was incomplete or contains errors, the assignments can be</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /0sers/mcortes/ptools-local/pgdbs/user/addedcyc/l.0/lnput/organism-init.dat Copying class Organisms from METABASE to ADDEDBASE. [Copyled class hierarchy into ADDEDBASE] [completed initialization of new PGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3654 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Save DB". Alternatively, the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SBML File" Command: Select and Read SEML File Reading SBML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SBML: 0 Number of Compartments in the SBML model: 2 Compartment ID Name (in SBML) Mapped to BioCyc CCO c cytosol cytosol e extracellular extracellular space After the SBML to the corresponding compartments in the BioCyc ontology.</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /USers/mcortes/ploofs-local/pgdbs/user/addedcyc/1.0/input/organism-Init.dat Copying class Organisms from METABASE to ADDEDBASE. [Completed initialization of new PGDB for ADDED] [Saving KB ADDEDBASE to V4-FRSL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 3564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel- t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Revert DB" vill undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/pesktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CCO c cytosol cytosol e extracellular extracellular space After the SEML file was read, the Importer tried to map the compartments described in SEML to the corresponding compartments in the BioCyc ontology. If this mapping was incomplete or contains errors, the assignments can be corrected with the command "Fix SEML Compartment Mapping"</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>Saved /OSerS/mcOrtes/ptools-local/pgubs/user/sddedcyc/l.0/input/organism-init.dat Copying class hierarchy into ADDEDBASE] [Completed initialization of new FGDE for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB FGDE-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CCO e cytosol cytosol e extracellular extracellular space After the SEML file was read, the Importer tried to map the compartments described in SEML to the corresponding compartments in the BioCyc ontology. If this mapping was incomplete or contains errors, the assignments can be</pre>				
Database rganism: RG-ID: ADD Name: *E. tatus: Modif te: Alog of all mess naole window can b seramocretex/SBML '11-29.txt Workflow Pro Read SBML Create comp Create speci	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>>swed /USETS/MCOTCES/PLOOTS-TOCAT/PGGDS/USET/AddedCyC/1.0/Input/Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDB for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Rever DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CC0 c cytosol e extracellular extracellular space After the SEML file was read, the Importer tried to map the compartments described in SEML to the corresponding compartments in the BioCyc ontology. If this mapping was incomplete or contains errors, the assignments can be corrected with the command "Fix SEML Compartment Mapping" The next suggested step is to run the command: </pre>				
Database rganism: RG-ID: ADD Vame: *E. tatus: Modif te: Alog of all mess socie window can b socie window can b restincortex/SBML 11-29.txt Workflow Prr Read SBML Create comp Create speci Merge comp	DED fied sages that appear in the se found in -Import-Console-Log-20 ogress: partments les and reactions oounds	<pre>>swed /USETS/MCOTCES/PLOOTS-TOCAT/PGGDS/USET/AddedCyC/1.0/Input/Organisms from METABASE to ADDEDBASE. [Copying class hierarchy into ADDEDBASE] [Completed initialization of new PGDB for ADDED] [Saving KB ADDEDBASE to V4-FASL file /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedba e.ocelot 0 frames ignored 9564 frames saved] [Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/FGDB-METADATA.ocel t 0 frames ignored 3 frames saved] After new changes have been made to the database, they can be saved by the command "Save DB". Alternatively, the command "Rever DB" will undo the changes by resetting the database to the previously saved contents. The next suggested step is to run the command "Import->Select and Read SEML File" Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml Number of (low-level) Errors reading SEML: 0 Number of Compartments in the SEML model: 2 Compartment ID Name (in SEML) Mapped to BioCyc CC0 c cytosol e extracellular extracellular space After the SEML file was read, the Importer tried to map the compartments described in SEML to the corresponding compartments in the BioCyc ontology. If this mapping was incomplete or contains errors, the assignments can be corrected with the command "Fix SEML Compartment Mapping" The next suggested step is to run the command: </pre>				

• <u>Step 5:</u> We ran the command "*Import->Create SBML Species (i.e. Compounds)* and *Reactions*". In this step, reactions from the MetaCyc database were

identified.

	-					
Database						
Organism:		ad SEML File /pgdbs/user/addedcyc/i.v/input/organism-init.dat BASE to ADDEDBASE.				
		artment Mapping EDBASE1				
Name: ^E.		ecies (= Compounds) and Reactions PGDB for ADDED] clas (= Compounds) ile /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/kb/addedbas				
	,	acres (- combounds)				
tatus: Modi	Merge SBML Re					
		9564 frames saved]				
		[[Saving KB PGDB-METADATA to V1-SEXPR file /Users/mcortes/ptools-local/pgdbs/user/PGDB-METADATA.ocel				
onsole window can k	isages that appear in the be found in	0 frames ignored				
Jsers/mcortes/SBMI 7-11-29.txt	L-Import-Console-Log-20	3 frames saved]				
		After new changes have been made to the database,				
		they can be saved by the command "Save DB".				
Workflow Pr	ourses!	Alternatively, the command "Revert DB" will undo the changes by resetting the database to the previously saved contents.				
WORKINGW I T	ogress.	resetting the database to the previously saved contents.				
Read SBML		The next suggested step is to run the command "Import->Select and Read SBML File"				
Create comp						
Merge comp	ies and reactions	Command: Select and Read SEML File Reading SEML file: /Users/mcortes/Desktop/added_AureMe_PadMet.xml				
Merge react		Number of (low-level) Errors reading SBML: 0				
•						
		Number of Compartments in the SEML model: 2				
		Compartment ID Name (in SBML) Mapped to BioCyc CCO				
		c cytosol cytosol e extracellular extracellular space				
		After the SBML file was read, the Importer tried to map the compartments				
		described in SEML to the corresponding compartments in the BioCyc ontology. If this mapping was incomplete or contains errors, the assignments can be				
		corrected with the command "Fix SBML Compartment Mapping"				
		The next suggested step is to run the command: "Import->Create SBML Species (= Compounds) and Reactions"				
		<u></u>				
		SBML Import				
Database	Import	IX SBML Import				
Database	Import	SBML Import				
Database)rganism :	-					
Database	-	Command: Create SBML Species (= Compounds) and Reactions				
Database Drganism: DRG-ID: ADE	-	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480				
Database Drganism: DRG-ID: ADE Name: *E.	DED	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) :				
Database Drganism: DRG-ID: ADE	DED	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol"				
Database Drganism: DRG-ID: ADE Name: *E.	DED	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) :				
Database Organism: DRG-ID: ADE Name: *E. Status: Modi	DED	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins				
Database Organism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes onsole window can b	DED fied sages that appear in the se found in	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0				
Database Organism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes onsole window can b	DED fied	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes onsole window can b Jears/mortes/SBMI	DED fied sages that appear in the se found in	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through NIL frames in Pathways class; de-duplicated citation count: 2 Searched through 267 frames in Datymatic-Reactions class; de-duplicated citation count: 2				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes onsole window can b Jears/mortes/SBMI	DED fied sages that appear in the se found in	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through NIL frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through 267 frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 1499 frames in Proteins class; de-duplicated citation count: 493				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes onsole window can b Jears/mortes/SBMI	DED fied sages that appear in the ce found in L-Import-Console-Log-20	Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through NIL frames in Pathways class; de-duplicated citation count: 2 Searched through NIL frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 1499 frames in Proteins class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674				
Database Drganism: DRG-ID: ADE Name: 'E. Status: Modi ote: A log of all mes oncode window can to Jearamoortes/SBMI -7-11-29.bt	DED fied sages that appear in the or found in -Import-Console-Log-20 ogress:	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through f19 frames in Pathways class; de-duplicated citation count: 2 Searched through NIL frames in Pathways class; de-duplicated citation count: 2 Searched through NIL frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 467 frames in DNA-Segments class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 196 frames in Organisms class; de-duplicated citation count: 1741				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes oracle window can be bereface the state of the state servincer the state of the state Workflow Pr I Read SBML	DED fied sages that appear in the oe found in I-import-Console-Log-20 ogress:	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 619 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through AIL frames in Datymatic-Reactions class; de-duplicated citation count: 2 Searched through 267 frames in DNA-Segments class; de-duplicated citation count: 433 Searched through 1499 frames in Oroteins class; de-duplicated citation count: 493 Searched through 27 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 196 frames in RNAs class; de-duplicated citation count: 1741 Searched through 1813 frames in RNAs class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mee onsole window can to Jesrahmortes/SBML 7-11-29.bt Workflow Pr Read SBML Create comp	DED fied sages that appear in the ce found in L-import-Console-Log-20 ogress: coartments	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 1619 frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through 267 frames in DRA-Segments class; de-duplicated citation count: 2 Searched through 4679 frames in Proteins class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 196 frames in RNAs class; de-duplicated citation count: 1674 Searched through 1813 frames in Frotein-Features class; de-duplicated citation count: 1742 Searched through 1813 frames in Royation class; de-duplicated citation count: 1742 Searched through 1611 frames in Compution-Faures class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci Create speci Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through NIL frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through NIL frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 467 frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 467 frames in DNA-Segments class; de-duplicated citation count: 493 Searched through 467 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 165 frames in NAS class; de-duplicated citation count: 1742 Searched through 181 frames in Protein-Features class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes onede window can the berrahmore window can the	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 1619 frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through 267 frames in DRA-Segments class; de-duplicated citation count: 2 Searched through 4679 frames in Proteins class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 196 frames in RNAs class; de-duplicated citation count: 1674 Searched through 1813 frames in Frotein-Features class; de-duplicated citation count: 1742 Searched through 1813 frames in Royation class; de-duplicated citation count: 1742 Searched through 1611 frames in Compution-Faures class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci Create speci Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through NIL frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through NIL frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through 1499 frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 4671 frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 1499 frames in Rotein-Features class; de-duplicated citation count: 1742 Searched through 181 frames in Frotein-Features class; de-duplicated citation count: 1742 Searched through 181 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 1 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci Create speci Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through A19 frames in Pathways class; de-duplicated citation count: 2 Searched through A19 frames in Pathways class; de-duplicated citation count: 2 Searched through A19 frames in Droteins class; de-duplicated citation count: 2 Searched through 4671 frames in Droteins class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-Rnd-Elements class; de-duplicated citation count: 1674 Searched through 27 frames in NRAs class; de-duplicated citation count: 1741 Searched through 1813 frames in RNAs class; de-duplicated citation count: 1742 Searched through 20 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 1 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through A17 frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through A267 frames in DNR-Segments class; de-duplicated citation count: 2 Searched through 4671 frames in DNR-Segments class; de-duplicated citation count: 1493 Searched through 477 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 477 frames in Proteins class; de-duplicated citation count: 1741 Searched through 1813 frames in Proteins class; de-duplicated citation count: 1742 Searched through 1813 frames in Protein-Features class; de-duplicated citation count: 1742 Searched through 1813 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 1 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Reactions imported from SEML : 278 of which there are 27 transport reactions				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 149 frames in Pathways class; de-duplicated citation count: 2 Searched through 149 frames in Proteins class; de-duplicated citation count: 2 Searched through 1491 frames in Proteins class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 27 frames in Compounds-And-Elements class; de-duplicated citation count: 1742 Searched through 196 frames in RNAs class; de-duplicated citation count: 1742 Searched through 191 frames in Grottin-Gaurisms class; de-duplicated citation count: 1742 Searched through 193 frames in Grottin-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Reactions imported from SEML : 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Bratways class; de-duplicated citation count: 2 Searched through 1499 frames in Bratways class; de-duplicated citation count: 2 Searched through 671 frames in Droteins class; de-duplicated citation count: 2 Searched through 4671 frames in Organisms class; de-duplicated citation count: 493 Searched through 4671 frames in Organisms class; de-duplicated citation count: 1674 Searched through 1813 frames in Roteins-delsen duplicated citation count: 1742 Searched through 1813 frames in Rotein-Features class; de-duplicated citation count: 1742 Searched through 1813 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 1 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 4 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 5 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 5 frames in Growth-Observations class; de-duplicated citation count: 1742				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 619 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through A19 frames in Pathways class; de-duplicated citation count: 2 Searched through A19 frames in Pathways class; de-duplicated citation count: 2 Searched through A199 frames in Droteins class; de-duplicated citation count: 2 Searched through 4671 frames in Droteins class; de-duplicated citation count: 173 Searched through 4671 frames in Compounds-Rnd-Elements class; de-duplicated citation count: 1674 Searched through 471 frames in Compounds-Rnd-Elements class; de-duplicated citation count: 1674 Searched through 1813 frames in Trotein-Features class; de-duplicated citation count: 1742 Searched through 1813 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Reactions imported from SEML: 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology.				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 149 frames in Pathways class; de-duplicated citation count: 2 Searched through 149 frames in Proteins class; de-duplicated citation count: 2 Searched through 1491 frames in Proteins class; de-duplicated citation count: 493 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 27 frames in Compounds-And-Elements class; de-duplicated citation count: 1742 Searched through 196 frames in RNAs class; de-duplicated citation count: 1742 Searched through 191 frames in Grottin-Gaurisms class; de-duplicated citation count: 1742 Searched through 193 frames in Grottin-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Grotth-Media class; de-duplicated citation count: 1742 Reactions imported from SEML : 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 149 frames in Pathways class; de-duplicated citation count: 2 Searched through 149 frames in Proteins class; de-duplicated citation count: 2 Searched through 149 frames in Droteins class; de-duplicated citation count: 1674 Searched through 27 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 1813 frames in Roteins class; de-duplicated citation count: 1741 Searched through 1813 frames in Roteins class; de-duplicated citation count: 1742 Searched through 1813 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 1 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Reactions imported from SEML : 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology. If a chemical compound occurs in several compartments, then in SEML, there exists a separate Species for each occurrance of the compound in a compartment. In BioCyc, on the other hand, there should be only				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 77 "extracellular space" > 2 bins are present; 480 total counts are in the bins Searched through 619 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through 619 frames in Proteins class; de-duplicated citation count: 2 Searched through 619 frames in Proteins class; de-duplicated citation count: 433 Searched through 619 frames in Organisms class; de-duplicated citation count: 1674 Searched through 196 frames in Organisms class; de-duplicated citation count: 1674 Searched through 196 frames in RNAs class; de-duplicated citation count: 1742 Searched through 196 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 1913 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 191 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 196 fram SEML : 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology. If a chemical compound occurs in several compartments, then in SEML, there exists a separate Species for each occurrance of the co				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SBML Species (= Compounds) and Reactions Compounds (= Species) imported from SBML : 480 Compartment distribution of the SBML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Patways class; de-duplicated citation count: 2 Searched through 149 frames in Patways class; de-duplicated citation count: 2 Searched through 149 frames in Proteins class; de-duplicated citation count: 2 Searched through 149 frames in Droteins class; de-duplicated citation count: 1674 Searched through 27 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 1813 frames in Proteins class; de-duplicated citation count: 1741 Searched through 1813 frames in RTAS class; de-duplicated citation count: 1742 Searched through 196 frames in Rome class; de-duplicated citation count: 1742 Searched through 1813 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Drotein-Searce class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Reactions imported from SEML : 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology. If a chemical compound occurs in several compartments, then in SEML, there exists a separate Species for each occurrance of the compound in a compartment. In BioCyc, on the other hand, there should be only				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 433 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 11 frames in Rathways class; de-duplicated citation count: 2 Searched through 11 frames in Pathways class; de-duplicated citation count: 2 Searched through 71 frames in DNA-Segments class; de-duplicated citation count: 493 Searched through 4671 frames in Proteins class; de-duplicated citation count: 493 Searched through 196 frames in Onganisms class; de-duplicated citation count: 1674 Searched through 196 frames in NTA-Segments class; de-duplicated citation count: 1674 Searched through 196 frames in Proteins-Features class; de-duplicated citation count: 1742 Searched through 196 frames in Royalisms class; de-duplicated citation count: 1742 Searched through 196 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Reactions imported from SEML : 278 of which there are 27 transport reactions At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology. If a chemical compound occurs in several compartments, then in SEML, there exists a separate Species for each occurrance of the compound in a compartment. In BioCyc, on the other hand, there should be only one compound frame, and the compartments are indica				
Database Drganism: DRG-ID: ADE Name: *E. Status: Modi ote: A log of all mes nacle window can b Jesrathwortex/SBML 7-11-29.bt Workflow Pr Read SBML Create speci Create speci	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	<pre>Command: Create SEML Species (= Compounds) and Reactions Compounds (= Species) imported from SEML : 480 Compartment distribution of the SEML Species (= Compounds) : 453 "cytosol" 27 "extracellular space" => 2 bins are present; 480 total counts are in the bins Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through NLI frames in Pathways class; de-duplicated citation count: 2 Searched through 1499 frames in NRA-Segments class; de-duplicated citation count: 2 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 4671 frames in Compounds-And-Elements class; de-duplicated citation count: 1674 Searched through 27 frames in Compounds-And-Elements class; de-duplicated citation count: 1742 Searched through 196 frames in RNAs class; de-duplicated citation count: 1744 Searched through 196 frames in Royation class; de-duplicated citation count: 1742 Searched through 196 frames in Royation class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742 Searched through 3 frames in Sextl file. Species correspond to compounds, in BioCyc terminology. If a chemical compound occurs in several compartments, then in SEML, there exists a separate Species for each occurrance of the compound in a compartment. In BioCyc, on the other hand, there should be only one compound frame, and the compartments are indicated in the reactions, instead. Thus, what needs to happen in the next steps is merging of the duplicate SEML Species into juut one compound frame. The next suggested step is to run the command:</pre>				
Database Prganism: PRG-ID: ADC Name: *E. Itatus: Modi ote: Alog of all mee anade window can be ensitive or text SBML '11-23.bt Workflow Pr Read SBML Create comp: Create speci Merge comp	DED fied sages that appear in the ce found in I-Import-Console-Log-20 ogress: partments les and reactions sounds	<pre>Improve the set of the set o</pre>				

• <u>Step 6:</u> We ran the command "Import->Merge SBML Species (i.e. Compounds)".

	SBML Import
Database Import	
organon.	ad SEML File
ORG-ID: ADE Fix SBML Comp	ompounds) and Reactions
	pecies (= Compounds) and Reactions om SEML : 480
Merge SBML Sp	ecies (= Compounds) BML Species (= Compounds) :
Status: Modi	actions
otatus: mouniou	27 "extracellular space"
	=> 2 bins are present; 480 total counts are in the bins
Note: A log of all messages that appear in the console window can be found in //Jershincortex/SBML-import-Console-Log-20 17-11-29.txt	Searched through 319 frames in Reactions class; de-duplicated citation count: 0 Searched through 619 frames in Pathways class; de-duplicated citation count: 2 Searched through NIL frames in Enzymatic-Reactions class; de-duplicated citation count: 2 Searched through 267 frames in DNA-Segments class; de-duplicated citation count: 2 Searched through 1499 frames in Proteins class; de-duplicated citation count: 493 Searched through 4671 frames in Proteins class; de-duplicated citation count: 494
Workflow Progress:	Searched through 27 frames in Organisms class; de-duplicated citation count: 1674 Searched through 196 frames in RNAs class; de-duplicated citation count: 1741
Read SBML Create compartments Create species and reactions Merge compounds Merge reactions	Searched through 1813 frames in Protein-Features class; de-duplicated citation count: 1742 Searched through 20 frames in Regulation class; de-duplicated citation count: 1742 Searched through 1 frames in Growth-Media class; de-duplicated citation count: 1742 Searched through 3 frames in Growth-Observations class; de-duplicated citation count: 1742
	Reactions imported from SEML : 270 of which there are 27 transport reactions
	At this stage, the Importer has created a frame for each SEML Species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology.
	If a chemical compound occurs in several compartments, then in SBML, there exists a separate Species for each occurrance of the compound in a compartment. In BioGyc, on the other hand, there should be only one compound frame, and the compartments are indicated in the reactions, instead. Thus, what needs to happen in the next steps is merging of the duplicate SEML Species into just one compound frame.
	The next suggested step is to run the command: "Import->Merge SBML Species (= Compounds)" 7
000	💢 SBML Import

Database Import	
Organism: ORG-ID: ADDED Name: *E.	And this stage, the importer has created a frame for each sphi species and Reaction, using the ID from the SEML file. Species correspond to compounds, in BioCyc terminology.
Status: Modified Note: A log of all messages that appear in the console window can be found in Usersmoorthes/SBML-import-Console-Log-20 7-11-29.btl	If a chemical compound occurs in several compartments, then in SEML, there exists a separate Species for each occurrance of the compound in a compartment. In BioCyc, on the other hand, there should be only one compound frame, and the compartments are indicated in the reactions, instead. Thus, what needs to happen in the next steps is merging of the duplicate SEML Species into just one compound frame. The next suggested step is to run the command: "Import->Merge SEML Species (= Compounds)"
Workflow Progress: Read SBML Create compartments	The next steps will try to match first the compounds and then the reactions with the corresponding frames in MetaCyc. Matched frames will be imported from MetaCyc and the verbatim SBML frames will be merged into the frames from MetaCyc, to reduce redundancies. Thereafter, in a later step, duplicate SBML reactions will need to be merged, likewise.
Create species and reactions Merge compounds Merge reactions	Command: Merge SEML Species (= Compounds) ;;; Collecting DBlinks: ;;; CollectIng DBlinks: a SEML. 8299 in MetaCyc. 0 not found in MetaCyc. ;;; LIGAND-CPD: 0 links in SEML. 6047 in MetaCyc. 0 not found in MetaCyc. ;;; INCHI: 1 links in SEML. 13452 in MetaCyc. 0 not found in MetaCyc.
	Details of compound merging can be found in: /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/reports/SEML-Import-Details-Log-2017-11-29.txt
	Surviving SBML Species (= compounds) after merges: 12
	Deleted 468 SBML Species during merger into 453 compounds, of which 441 were imported from MetaCyc.
	The next suggested step is to run the command: "Import->Merge SBML Reactions"

			X SBML Import		
Database Import					
Organism: ORG-ID: ADDED Name: *E.	;;; LIGAND-CPD: 0	links: links in SBML. links in SBML.	pounds; 8299 in MetaCyc. 0 not foun 6047 in MetaCyc. 0 not foun 13452 in MetaCyc. 0 not fou	d in MetaCyc.	
Status: Modified		nd merging can be tools-local/pgdbs	found in: /user/addedcyc/1.0/reports/SBN	ML-Import-Deta	ails-Log-2017-11-29.tz
Note: A log of all messages that appear in the console window can be found in /Users/mcortes/SBML-Import-Console-Log-20 17-11-29.txt			s) after merges: 12		
Workflow Progress:		e imported from M			
Read SBML	"Import->Merge S		the command.		
Create compartments Create species and reactions Merge compounds Merge reactions	Command: Merge SE ;;; Collecting DE ;;; DBlink->Rxn h ;;; KEGG (RXN): C	links: ash-tables:	4894 in MetaCyc. O not found	d in MetaCyc.	
	Details of reacti /Users/mcortes/p		found in: /user/addedcyc/1.0/reports/SB	ML-Import-Deta	ails-Log-2017-11-29.tz
			TOSOL to the RXN-LOCATIONS of TOSOL to the RXN-LOCATIONS of		
	Starting SBML Rea Surviving SBML Re				
	of which 183 wer SBML Reactions me	e imported from M rged into MetaCyc	merger into 276 surviving read letaCyc. Reactions, due to ignoring p Reactions, due to matches by	rotonation dif	

• <u>Step 8:</u> Finally, we saved our new **addedcyc** PGDB by running the command *"Database->Save DB"*.

	X SBML Import
Database Import	
Select an Existing Datab	base 1: merge somt spectes (- compounds)
Create a New Database	Llecting DBlinks:
Save DB	BBI: 0 links in SBML. 8299 in MetaCyc. 0 not found in MetaCyc. SAND-CPD: 0 links in SBML. 6047 in MetaCyc. 0 not found in MetaCyc.
Revert DB	CHI: 1 links in SML. 13452 in MetaCyc. 0 not found in MetaCyc.
Exit Note: A log of all messages that appear in the console window can be found in Usershnoortes/SML-Import-Console-Log-20 17-11-20.bt	Details of compound merging can be found in: /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/reports/SEML-Import-Details-Log-2017-11-29.txt Surviving SEML Species (= compounds) after merges: 12 Deleted 468 SEML Species during merger into 453 compounds.
Workflow Progress:	of which 441 were imported from MetaCyc. The next suggested step is to run the command:
	"Import->Merge SBML Reactions"
Read SBML	
Create compartments Create species and reactions Merge compounds Merge reactions	Command: Merge SEML Reactions ;;; Collecting DBlinks: ;;; DBlink->Rxn hash-tables: ;;; KEGG (RXN): 0 links in SEML. 4894 in MetaCyc. 0 not found in MetaCyc.
	Details of reaction merging can be found in: /Users/mcortes/ptools-local/pgdbs/user/addedcyc/1.0/reports/SEML-Import-Details-Log-2017-11-29.txt - Added CCO-EXTRACELLULAR-CCO-CYTOSOL to the RXN-LOCATIONS of "TRANS-RXN-185" - Added CCO-EXTRACELLULAR-CCO-CYTOSOL to the RXN-LOCATIONS of "TRANS-RXN-171"
	Starting SBML Reactions before merger: 278 Surviving SBML Reactions after merger: 93
	Deleted 185 SBML Reactions during merger into 276 surviving reactions, of which 183 were imported from MetaCyc. SBML Reactions merged into MetaCyc Reactions, due to ignoring protonation differences: 0 SBML Reactions merged into MetaCyc Reactions, due to matches by substrates: 185

3) In Pathway Tools v 21.0 we exported all reactions in our newly created PGDB (addedyc) to a Lispformat File. To do this, we started Pathway Tools though the Lisp interpreter with the following command:

• ./Pathway Tools -lisp

Then, we selected our addedcyc PGDB and exported all reactions to the file "added_frames.txt" with the following commands:

• (select-organism :org-id 'added)

• (export-frames-to-file nil "/PATH-TO-FILE/added_frames.txt" nil :classes '(|Reactions|))

Where "/PATH-TO-FILE/" is the directory where we stored our frames file added_frames.txt.

4) Then, we selected our original ectocyc2.2 PGDB and we opened the Pathway Tools GUI interface:

• (select-organism :org-id 'ectov2.2)

• (pt)

5) Finally, we imported the new reactions in "added_frames.txt" into ectocyc2.2 running the command:

• File->Import->Frames-from-Lisp-format File

The resulting PGDB is available online: ectov2.2cyc 1.0 in esiliculosus_PGDBs on http://aureme.genouest.org/suppdata.html

Bibliography

- Hucka,M., Finney,A., Sauro,H.M., Bolouri,H., Doyle,J.C., Kitano,H., Arkin,A.P., Bornstein,B.J., Bray,D., Cornish-Bowden,A., *et al.* (2003) The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models. *Bioinformatics*, **19**, 524– 31.
- 2. Karp,P.D., Paley,S. and Romero,P. (2002) The Pathway Tools software. *Bioinformatics*, **18**, S225--S232.
- 3. Loira,N., Zhukova,A. and Sherman,D.J. (2015) Pantograph: A template-based method for genomescale metabolic model reconstruction. *J. Bioinform. Comput. Biol.*, **13**, 1550006.
- 4. Li,L., Stoeckert,C.J., Roos,D.S. and Roos,D.S. (2003) OrthoMCL: identification of ortholog groups for eukaryotic genomes. *Genome Res.*, **13**, 2178–89.
- 5. Remm,M., Storm,C.E. V and Sonnhammer,E.L.L. (2001) Automatic clustering of orthologs and inparalogs from pairwise species comparisons. *J. Mol. Biol.*, **314**, 1041–1052.
- 6. Ebrahim,A., Lerman,J.A., Palsson,B.O. and Hyduke,D.R. (2013) COBRApy: COnstraints-Based Reconstruction and Analysis for Python. *BMC Syst. Biol.*, **7**, 74.
- 7. Steffensen, J.L., Dufault-Thompson, K. and Zhang, Y. (2016) PSAMM: A Portable System for the Analysis of Metabolic Models. *PLoS Comput. Biol.*, **12**, e1004732.

- Prigent,S., Frioux,C., Dittami,S.M., Thiele,S., Larhlimi,A., Collet,G., Gutknecht,F., Got,J., Eveillard,D., Bourdon,J., *et al.* (2017) Meneco, a Topology-Based Gap-Filling Tool Applicable to Degraded Genome-Wide Metabolic Networks. *PLOS Comput. Biol.*, **13**, e1005276.
- Satish Kumar,V., Dasika,M.S., Maranas,C.D., Wei,J., Goldberg,M., Burland,V., Venkatesan,M., Deng,W., Fournier,G., Mayhew,G., *et al.* (2007) Optimization based automated curation of metabolic reconstructions. *BMC Bioinformatics*, **8**, 212.
- 10. Thiele,I., Vlassis,N. and Fleming,R.M.T. (2014) fastGapFill: efficient gap filling in metabolic networks. *Bioinformatics*, **30**, 2529–2531.
- Schellenberger, J., Que, R., Fleming, R.M.T., Thiele, I., Orth, J.D., Feist, A.M., Zielinski, D.C., Bordbar, A., Lewis, N.E., Rahmanian, S., *et al.* (2011) Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox v2.0. *Nat. Protoc.*, 6, 1290–307.
- Agren,R., Liu,L., Shoaie,S., Vongsangnak,W., Nookaew,I. and Nielsen,J. (2013) The RAVEN Toolbox and Its Use for Generating a Genome-scale Metabolic Model for Penicillium chrysogenum. *PLoS Comput. Biol.*, **9**, e1002980.
- Shannon,P., Markiel,A., Ozier,O., Baliga,N.S., Wang,J.T., Ramage,D., Amin,N., Schwikowski,B. and Ideker,T. (2003) Cytoscape: a software environment for integrated models of biomolecular interaction networks. *Genome Res.*, **13**, 2498–2504.