Reactome

Export of BioPax and SBML from Reactome

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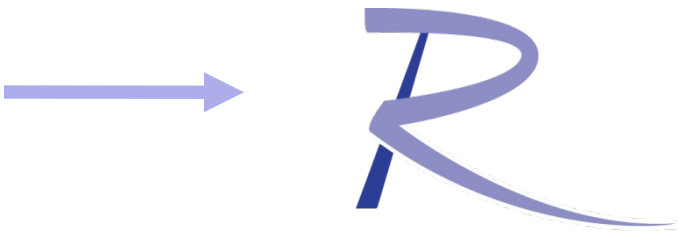
EMBL-EBI CSH

Rationale – Journal information

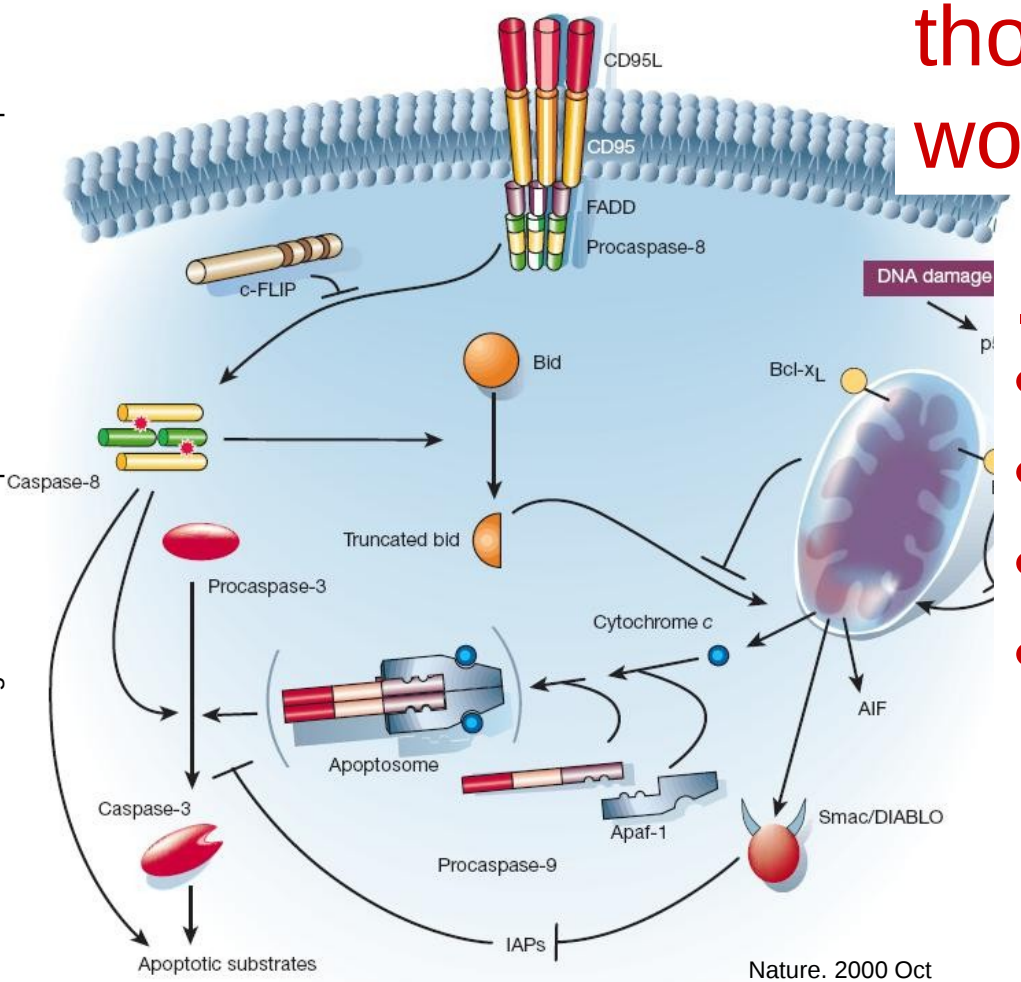
Nature 407(6805):770-6.The Biochemistry of Apoptosis.

"Caspase-8 is the key initiator caspase in the death-receptor pathway. Upon ligand binding, death receptors such as CD95 (Apo-1/Fas) aggregate and form membrane-bound signalling complexes (Box 3). These complexes then recruit, through adapter proteins, several molecules of procaspase-8, resulting in a high local concentration of zymogen. The induced proximity model posits that under these crowded conditions, the low intrinsic protease activity of procaspase-8 (ref. 20) is sufficient to allow the various proenzyme molecules to mutually cleave and activate each other (Box 2). A similar mechanism of action has been proposed to mediate the activation of several other caspases, including caspase-2 and the nematode caspase CED-3 (ref. 21)."

How can I access the pathway described here and reuse it?



Rationale - Figures



Nature. 2000 Oct 12;407(6805):770-6.
The biochemistry of apoptosis.

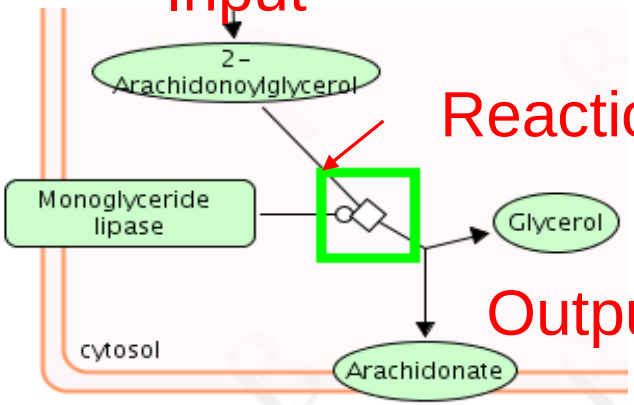
A picture paints a thousand words…

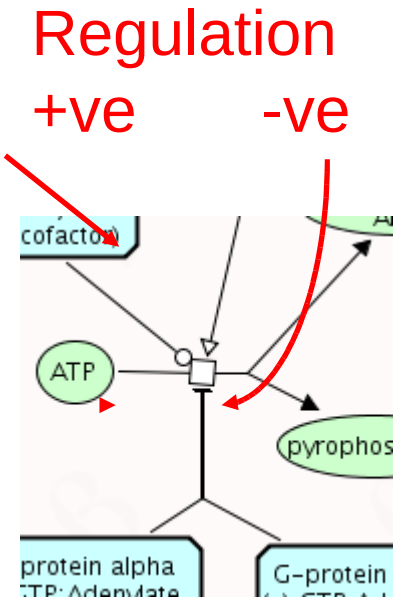
...but:

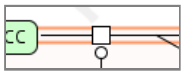
- Just pixels
- Omits key details
- Assumes
- Fact or Hypothesis?

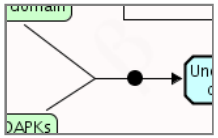
Events – reactions and regulations

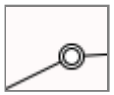
Boxes are proteins, protein sets, mixed sets or complexes.
Ovals are small molecules (or sets of)
Green boxes are proteins or sets, blue are complexes.

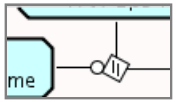


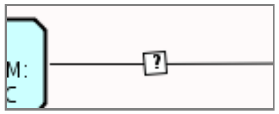



Transition

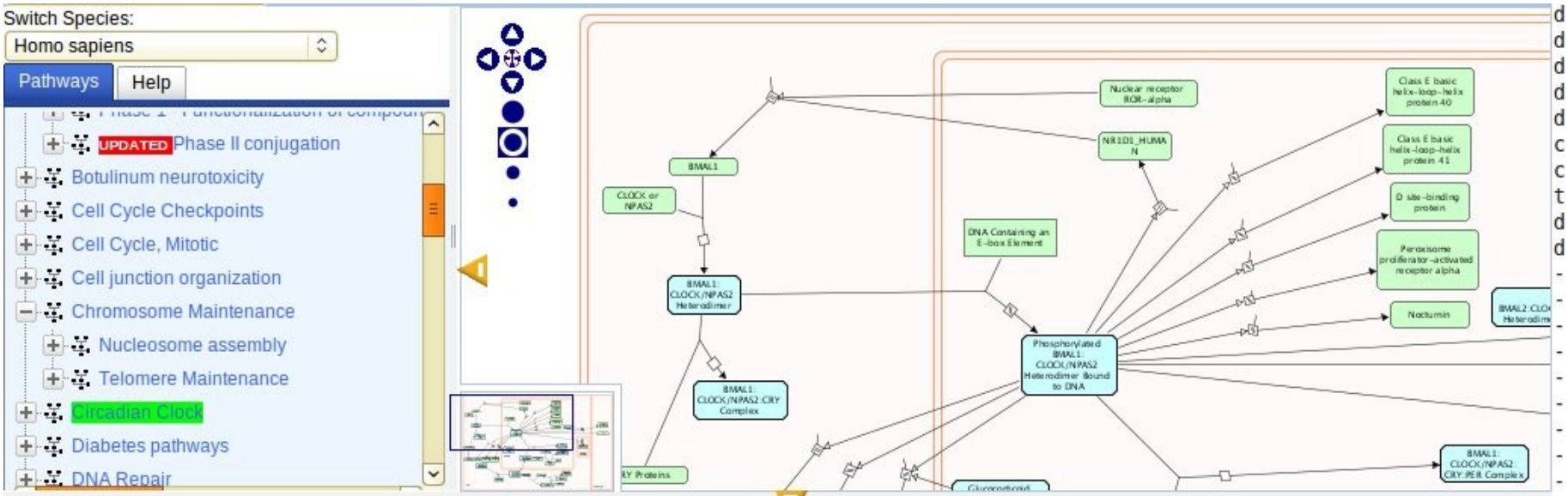

Binding


Dissociation


Omitted


Uncertain

Events - pathways

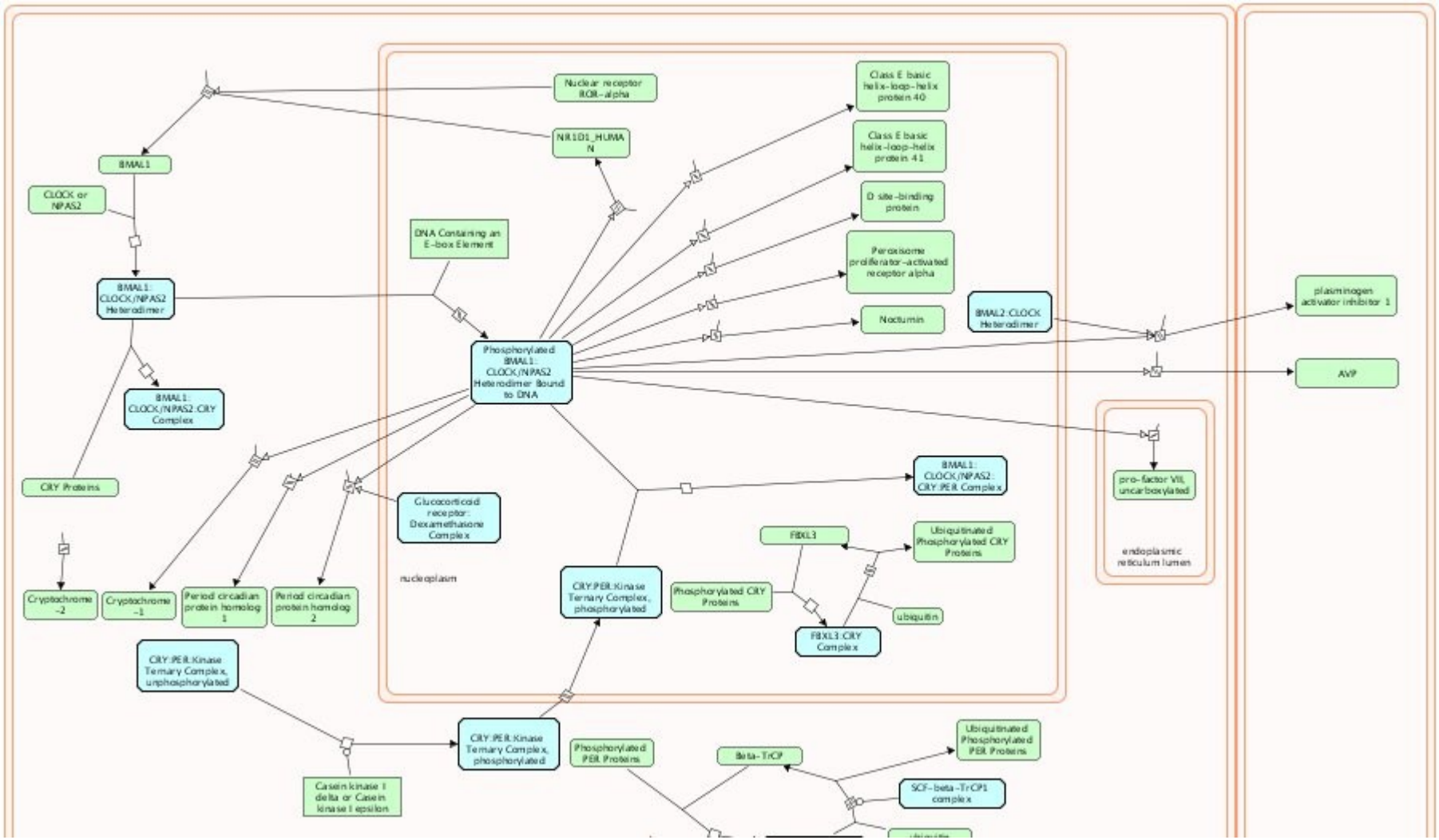


Circadian Clock

DOI	10.3180/REACT_24941.1
Stable identifier	REACT_24941.1
Authored	May, B, 2009-05-17
Reviewed	D'Eustachio, P, 2009-05-26 Albrecht, U, 2010-06-23 Kay, SA, 2010-06-23 Hirota, T, 2010-06-23 Delaunay, F, 2010-06-23

At the center of the mammalian circadian clock is a negative transcription/translation-based feedback loop: The BMAL1:CLOCK/NPAS2 heterodimer transactivates CRY and PER genes by binding E-box elements in their promoters; the CRY and PER proteins then inhibit transactivation by BMAL1:CLOCK/NPAS2. BMAL1:CLOCK/NPAS2 activates transcription of CRY, PER, and several other genes in the morning. Levels of PER and CRY proteins rise during the day and inhibit expression of CRY, PER, and other BMAL1:CLOCK/NPAS2-activated genes in the afternoon and evening. During the night CRY and PER proteins are targeted for degradation by phosphorylation and polyubiquitination, allowing the cycle to commence

Manually laid-out pathway diagrams



Coverage

- Apoptosis
- Cell cycle
- DNA repair
- Transcription, mRNA processing, translation, post-translational modification
- Signaling pathways (insulin, NOTCH, opioid, NGF, EGFR, FGFR, Rho GTPases II, Opioid, Wnt)
- Hemostasis
- Metabolism (energy, amino acid, lipid, nucleotide, xenobiotic)
- Synaptic transmission
- Lipoproteins – HDL and VLDL

BioPax Output

- BioPax level 2 and level 3 provided.
- Available for single pathways or for the whole database.
- OWL format dump files.
- Under level 3, the following are exported:
  - bp:Pathway (pathway name)
  - bp:pathwayComponent (reactions)
  - bp:comment (text description)
  - bp:xref (Pubmed references)
  - bp:cellularLocation
  - bp:entityReference (Protein UniProt ID)
  - bp:UnificationXref (GO terms)

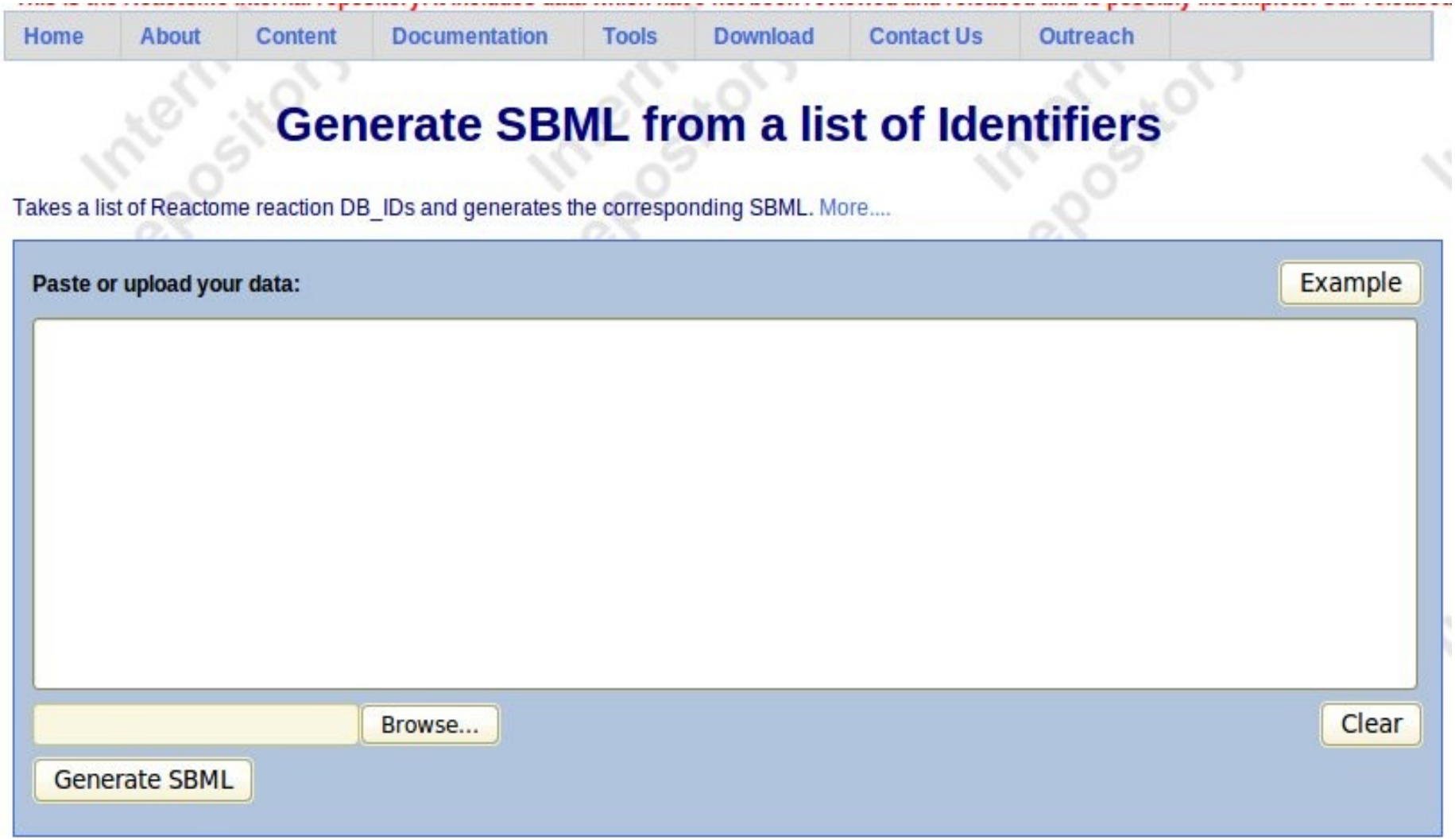
New SBML Output

- SBML level 2.3.
- Available for single pathways or for the whole database.
- Uses MIRIAM-compliant URIs for references to UniProt etc.
- The following are included in the SBML:
  - Coordinates for reactions, using layout extension.
  - listOfSpecies
  - ListOfCompartments
  - ListOfReactions
  - UniProt IDs, ChEBI IDs, GO Ids, PubMed IDs
  - Curated text summaries for reactions & pathways

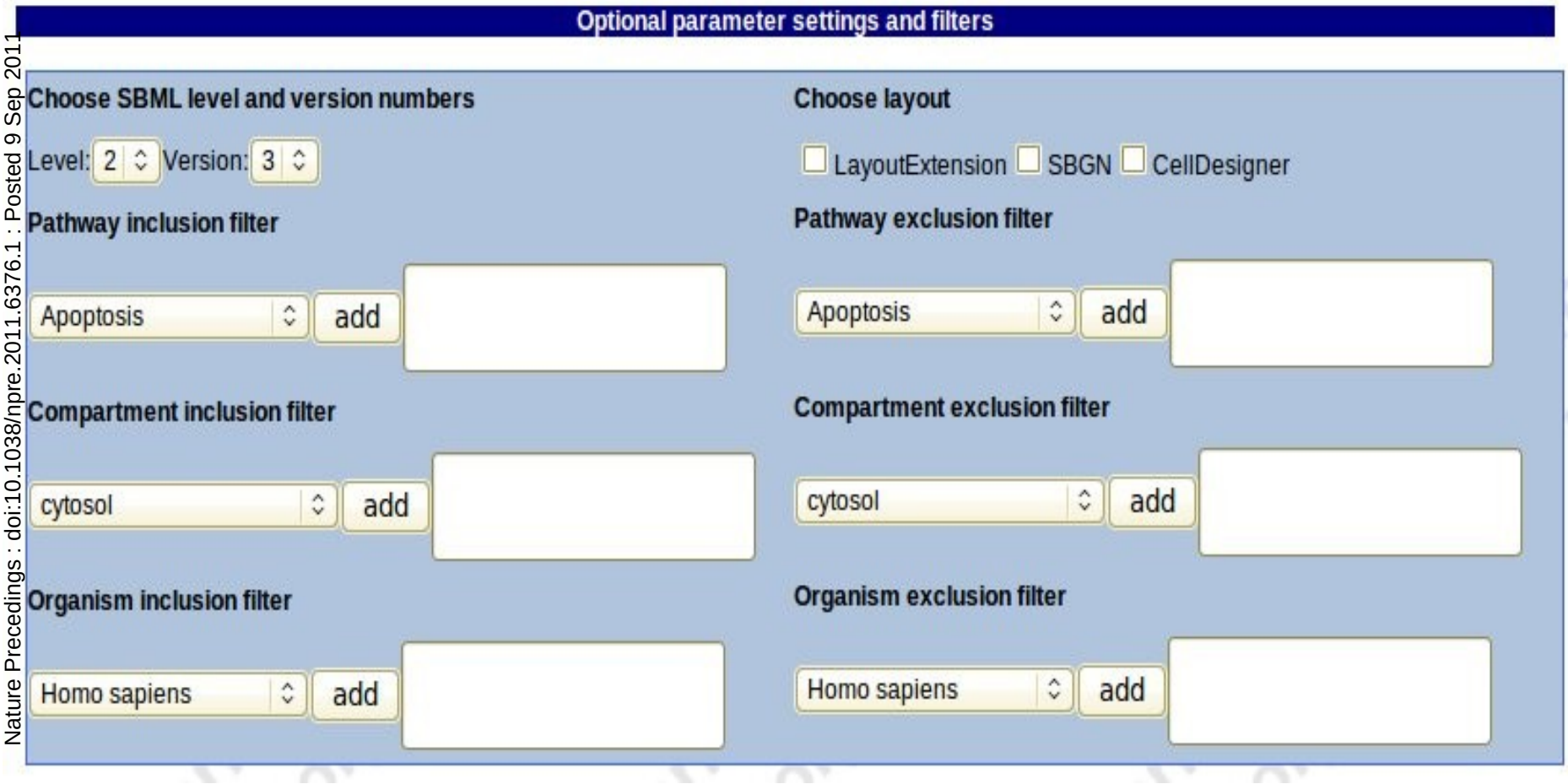
Future Plans

- RESTful API to allow custom query of Reactome, results returned as BioPax or SBML.
- Import reaction dynamics from other databases.
- Optional collapse of reactions.
- Interactive construction of SBML or BioPax based on user data.
- CellDesigner SBML
- Integration with systems biology packages, e.g. SBW??

Interactactive export of SBML or BioPax I



Interactactive export of SBML or BioPax II



Interactactive export of SBML or BioPax III

Select format to download this table: Microsoft Xcel Download

Pathway name	Species	Total number of proteins	Matching proteins in data	% in data	Click button to view pathway
ABC-family proteins mediated transport	Homo sapiens	15	0	0%	View
Adaptive Immunity Signaling	Homo sapiens	0	0	0%	View
Advanced glycosylation endproduct receptor signaling	Homo sapiens	13	1	7%	View
Amyloids	Homo sapiens	28	3	10%	View
APC/C-mediated degradation of cell cycle proteins	Homo sapiens	79	39	49%	View
Apoptosis	Homo sapiens	0	0	0%	View
Apoptotic execution phase	Homo sapiens	48	3	6%	View
Aquaporin-mediated transport	Homo sapiens	30	0	0%	View
Asparagine N-linked glycosylation	Homo sapiens	85	1	1%	View
Axon guidance	Homo sapiens	0	0	0%	View
Base Excision Repair	Homo sapiens	19	18	94%	View
Bile acid and bile salt metabolism	Homo sapiens	27	1	3%	View