Qualitative Bio Knowledge on Web

- Project by BioModels.net, curator Nick Juty
- Comprehensive collection of SB-relevant terms, hierarchical
- Includes terms for many rate laws, parameters and quantities
- For rate laws, includes math expression and references to SBO terms of the parameters (e.g. term for Michaelis-Menten rate law refers to term for Michaelis constant)

How to get the molecular weight

- For most common:
  - Hardcode weight, e.g. for ATP, Ca, GTP
  - Download from ChEBI
  
- Proteins:
  - Get sequence from UniProt
  - Calculate weight from sequence
  - Add modifications (e.g. phosphorylations)

Systems Biology Pathway Exchange (SBPAX)

- Integrated with BioPAX classes
- Extension to BioPAX L3 as SBPAX3
- Proposal for BioPAX L4
- Arranges Systems Biology terms (e.g. Systems Biology Ontology), numbers and units into hierarchies
- Units based on Units of Measurement Expressions (UOME)

Virtual Cell (Model View)

Virtual Cell (Pathway View)

Systems Biology Ontology (SBO)

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Quantitative Bio versus Modeling

- Model = Biology + Method
- Biology: biological reality; qualitative + quantitative; general + specific (=> BioPAX, SBPAX)
- Method: cropping, filtering, merging, requirements, assumptions, simplifications, omissions, artifacts (=> VCell)
- Model: Math (=> SBML, CellML)

Biological Details → Complete Knowledge
Knowledge → Computer-processable
Knowledge → Public
Computers → Much faster
Bio Models → Complete Biochem Details
Model Building → Automatic
Model Builder → Knowledgebase Frontend

Trends

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Bio Knowledge from Web into VCell

- Systems Biology Linker (SyBiL) at VCell: Grab Bio Knowledge from Web to build and annotate models
- Qualitative: Queries Pathway Commons, UniProt, ChEBI; imports BioPAX (since years)
- Quantitative: SBPAX3 from SGMP, SABIO-RK

Using the VCell Model DB

- Create statistics of all public models (some filtering)
- Classify by compartments, species, reactions
- Group species by ChEBI classes and UniProt keywords
- Find correlations between compartment sizes, initial conditions, kinetic parameters
- To create new models, find similar existing models, calculate numbers based on patterns/correlations.

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- SABIO-RK: Wolfgang Mueller, Martin Golebiewski, Ulrike Wittig, Renate Kania, Lenneke Jong, Enkhjargal Alga