

BioModels Database

<http://www.ebi.ac.uk/biomodels>

Chen Li

chenli@ebi.ac.uk

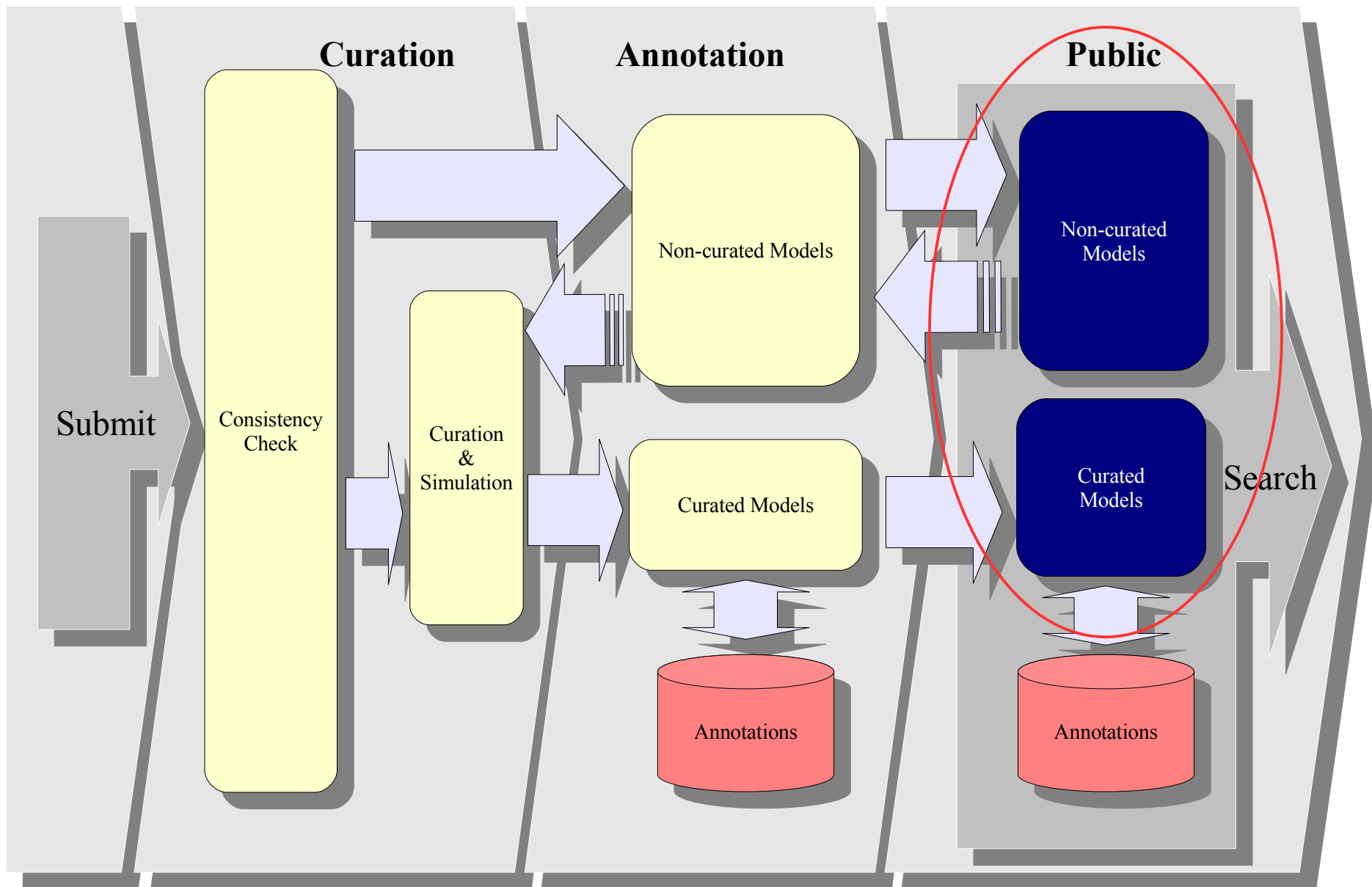
Insight BioModels Database

- **Apache Xindice**
- MySQL 4.1
- JSP, Java Bean
- libSBML
- Network layout and Application Server (Tomcat)
- External resources
- MIRIAM
- Other formats conversion

Insight BioModels Database

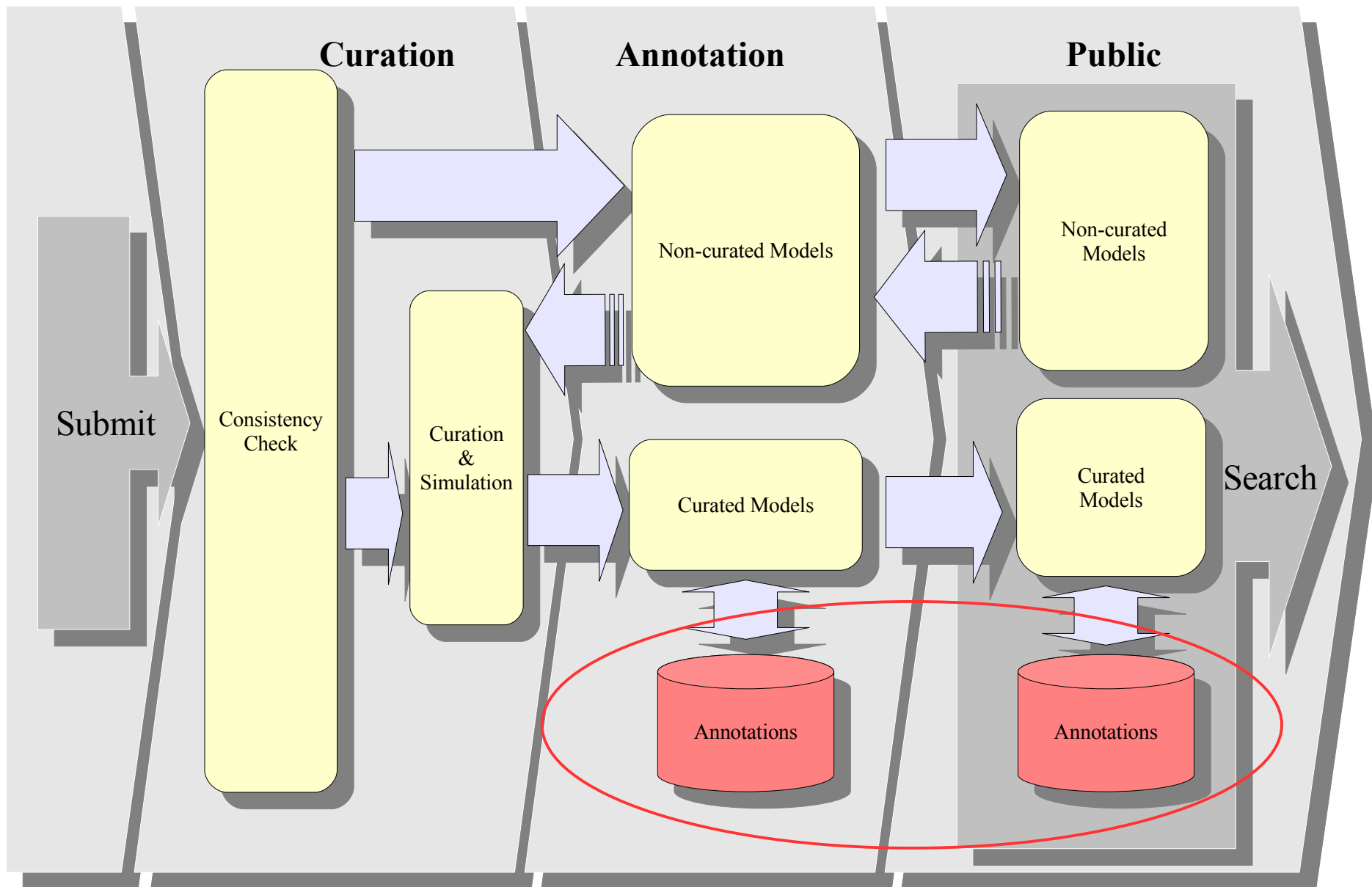
Native XML database (Xindice)

- **All SBML files are stored in Xindice.**
- **For very complex model, we don't have to map XML structure to other database.**
- **Xindice create index for the stored SBML files**
- ***Xpath* for query language;**
- ***XML:DB Update* for update language;**
- ***XML:DB API* for Java development.**



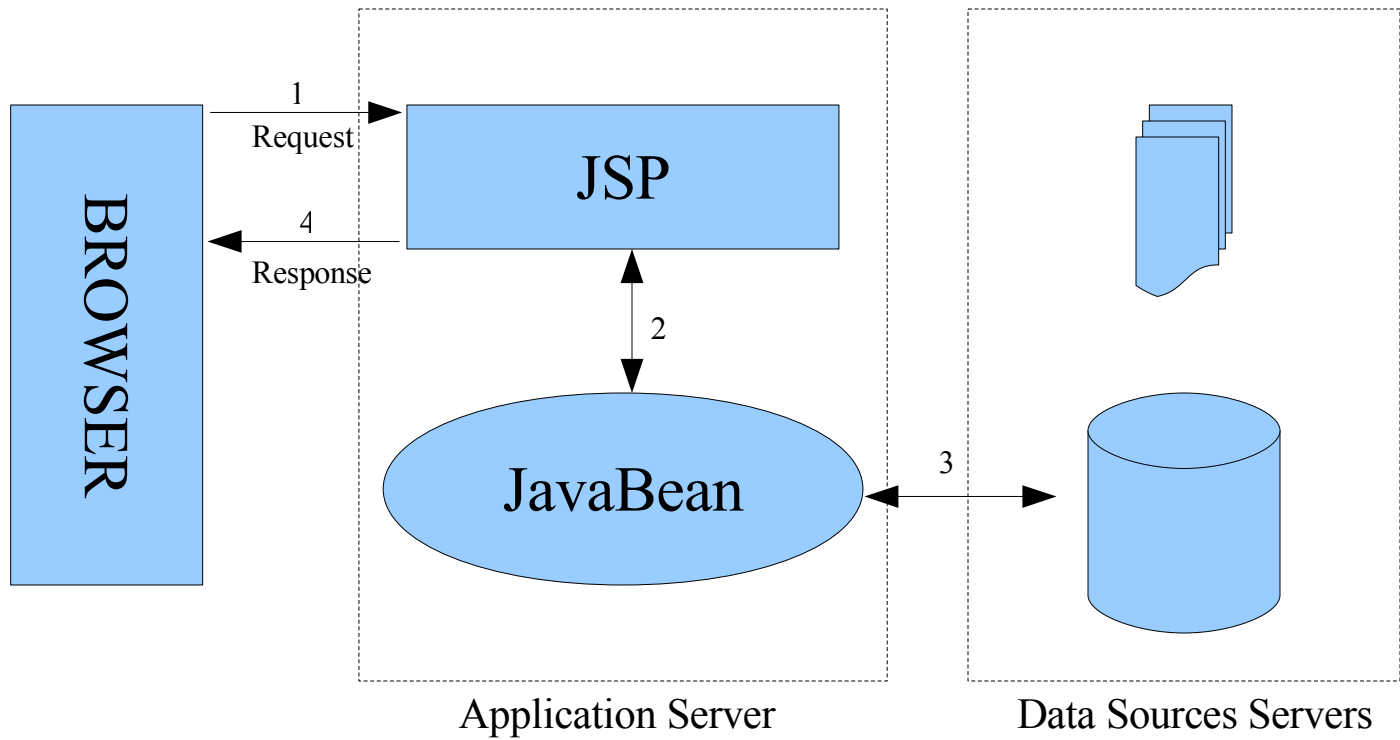
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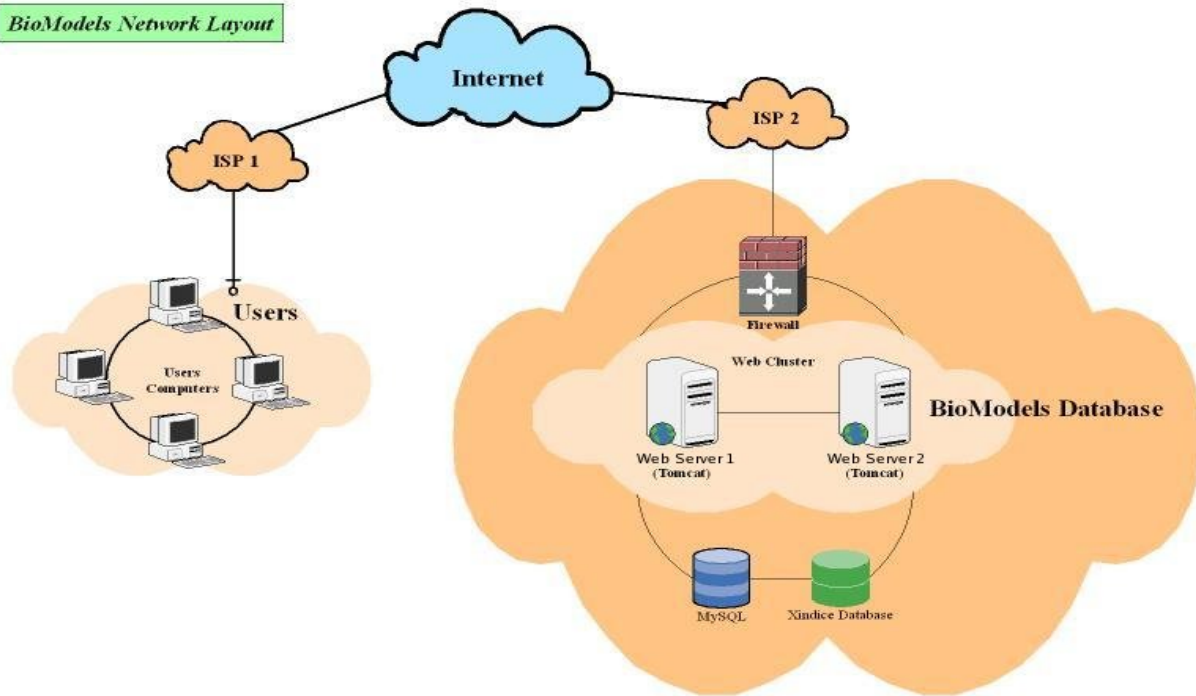
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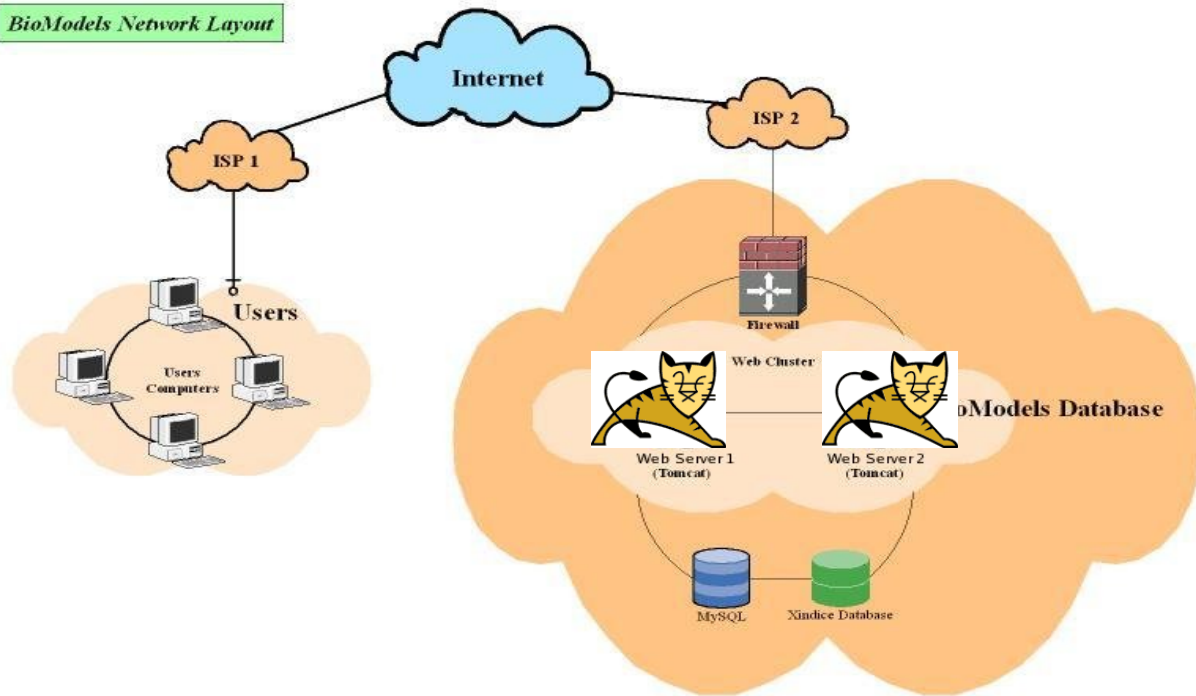
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BioModels Network Layout



BioModels Network Layout



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Insight BioModels

External resources

model	Submitter, Creators, <u>publication</u> , Gene Ontology, ICD10, KEGG pathway, OMIM, Reactome, Taxonomy
compartment	Gene Ontology
reaction participant	BIND complex, <u>ChEBI</u> , Ensembl, Gene Ontology, InterPro, KEGG compound, OMIM, <u>Taxonomy, UniProt</u>
mathematical expression	BIND interaction, EC code, Gene Ontology, IntAct, KEGG pathway, KEGG Reaction, Reactome

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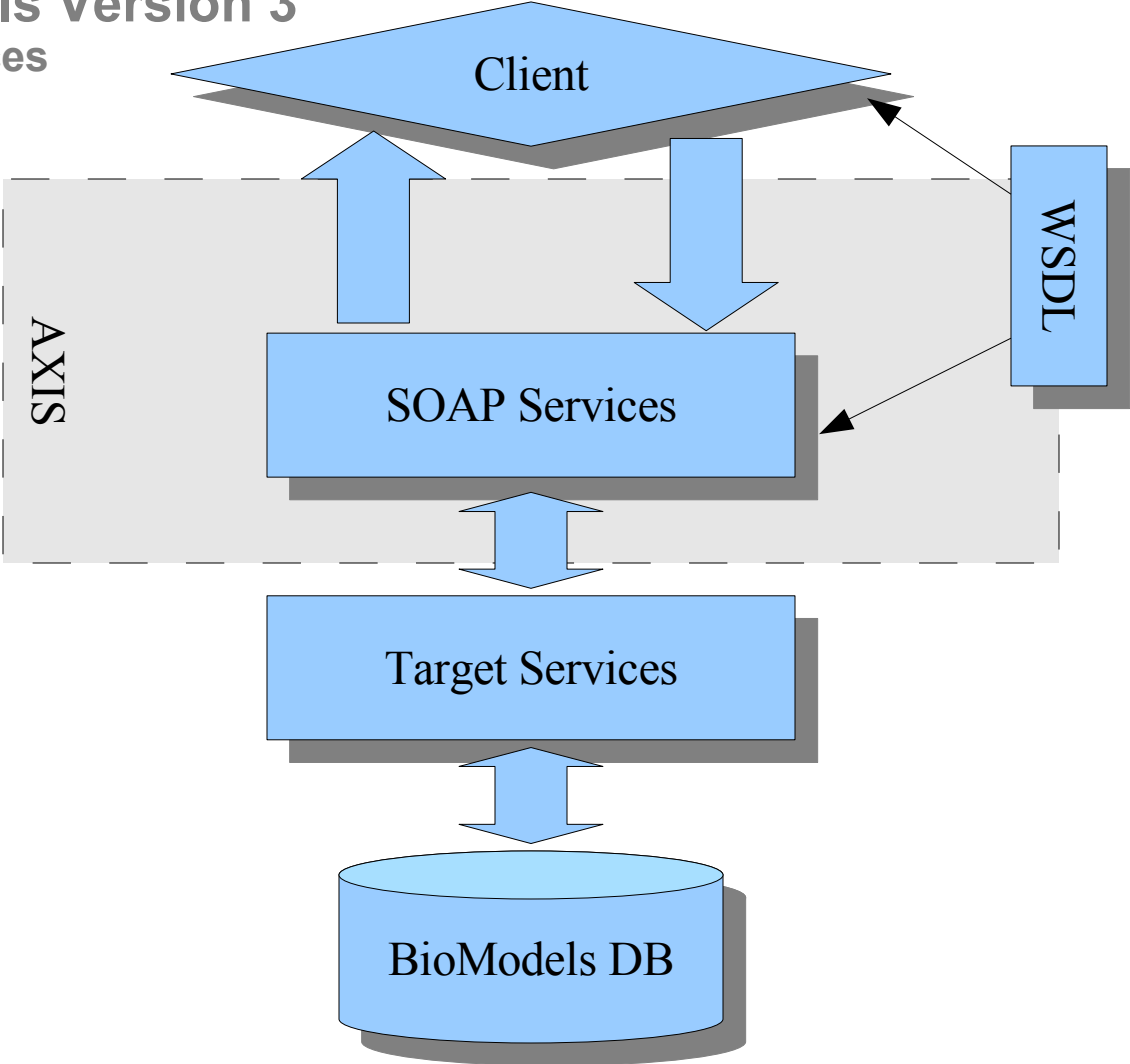
BioModels Version 3

- **SBML L2V2**
- Web Services
- Integrate other SBML softwares with BioModels DB
- Integration with SBO
- Interface improvement (AJAX)
- Relational database

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**BioModels Version 3
Web Services**



BioModels Version 3

Web Services developed

- String helloBioModels()**
- String getModelById(String modelId)**
- String getModelNameById(String modelId)**
- String[] getModelIdsByName(String modelName)**
- String[] getModelIdsByPublication(String publicationIdOrText)**
- String[] getModelIdsByPerson(String personName)**

BioModels Version 3
Web Services planning

Brainstorming

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[SBML L2 V1](#) | [CellML](#) | [SciLab](#) | [XPP](#) | [BioPAX](#)

[View Model Graph](#) | [View Model SVG](#) | [View Model Applet Graph](#)

[Submit Model Comment/Bug](#)

Reference Publication

Publication ID: [1831270](#)

Proc Natl Acad Sci U S A 1991 Aug;88(16):7328-32.
 Modeling the cell division cycle: cdc2 and cyclin interactions.
 Tyson JJ.
 Department of Biology, Virginia Polytechnic Institute and State University, Blacksburg 24061. [\[more\]](#)

Model

Original Model: *Unspecified*

Submitter: [Nicolas Le Novere](#)

Submission Date: 2005-09-13T13:31:08

Last Modification Date: 2006-04-02T18:20:03

Creation Date: 2005-02-08T18:28:27

Creators: [Bruce Shapiro](#)

bqbiol:is set #1 [Gene Ontology](#) [mitotic cell cycle](#)
[KEGG Pathway](#) [sce04110](#)
[Reactome](#) [69278](#)
[Taxonomy](#) [Fungi/Metazoa_group](#)

Compartments (1)

cell
Referred to as: cell bqbiol:is set #1 [Gene Ontology](#) [cell](#)

Species (7)

EmptySet
 Compartment: [cell](#)
Referred to as: EmptySet

cdc2k bqbiol:isVersionOf set #1 [UniProt](#) [CDC2_SCHPO](#)
 Compartment: [cell](#)
Referred to as: C2

cdc2k-P bqbiol:isVersionOf set #1 [UniProt](#) [CDC2_SCHPO](#)
 Compartment: [cell](#)
Referred to as: CP

p-cyclin_cdc2 bqbiol:hasPart set #1 [InterPro](#) [IPR006670](#)
[UniProt](#) [CDC2_SCHPO](#)
 Compartment: [cell](#)
Referred to as: M

p-cyclin_cdc2-p bqbiol:hasPart set #1 [InterPro](#) [IPR006670](#)
[UniProt](#) [CDC2_SCHPO](#)
 Compartment: [cell](#)
Referred to as: pM

cyclin bqbiol:isVersionOf set #1 [InterPro](#) [IPR006670](#)
 Compartment: [cell](#)
Referred to as: Y

p-cyclin bqbiol:isVersionOf set #1 [InterPro](#) [IPR006670](#)
 Compartment: [cell](#)

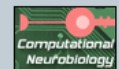


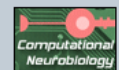
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BIOMODELS.NET





Reference Publication ⌵ ⌶ ⌷

Publication ID: [1833774](#) [Edit](#)
 Proc Natl Acad Sci U S A 1991 Oct;88(20):9107-11.
 A minimal cascade model for the mitotic oscillator involving cyclin and cdc2 kinase.
 Goldbeter A.
 Faculté des Sciences, Université Libre de Bruxelles, Belgium. [\[more\]](#)

Model ⌵ ⌶ ⌷

Original Model: *Unspecified* [Edit](#)
Submitter: [Nicolas Le Novère](#)
Submission Date: 2005-09-13T13:24:56
Last Modification Date: 2006-09-06T23:26:41
Creation Date: 2005-02-06T23:39:40
Creators: [Bruce Shapiro](#) [Remove](#)
[Add](#)

bqbiol:is	set #1	Taxonomy Amphibia Remove
Update	Gene Ontology	GO: <input type="text"/> Add Home
bqbiol:isVersionOf	set #1	Gene Ontology mitotic cell cycle Remove
Update	KEGG Pathway hsa04110 Remove	
bqbiol:isHomologTo	set #1	Reactome REACT_152 Remove
Update	Gene Ontology	GO: <input type="text"/> Add Home
bqmodel:is	Gene Ontology	GO: <input type="text"/> Add Home

Compartments (1) ⌵ ⌶ ⌷

cell ⊞
Referred to as: cell

bqbiol:is	set #1	Gene Ontology cell Remove
Update	Gene Ontology	GO: <input type="text"/> Add Home
bqmodel:is	Gene Ontology	GO: <input type="text"/> Add Home

Species (3) ⌵ ⌶ ⌷

Cyclin ⊞
 Compartment: *cell*
Referred to as: C

bqbiol:isVersionOf	set #1	InterPro IPR006670 Remove
Update	CHEBI	CHEBI: <input type="text"/> Add Home
bqmodel:is	CHEBI	CHEBI: <input type="text"/> Add Home

CDC-2 Kinase ⊞
 Compartment: *cell*
Referred to as: M

bqbiol:hasVersion	set #1	UniProt CDC2B_XENLA Remove
Update	UniProt CDC2A_XENLA Remove	
bqmodel:is	CHEBI	CHEBI: <input type="text"/> Add Home
bqmodel:is	CHEBI	CHEBI: <input type="text"/> Add Home

Cyclin Protease ⊞
 Compartment: *cell*
Referred to as: X

bqmodel:is	CHEBI	CHEBI: <input type="text"/> Add Home
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Rules (2) ⌵ ⌶ ⌷

Assignment Rule ⊞
Assignment Rule ⊞

bqmodel:is	Enzyme Nomenclature	<input type="text"/> Add Home
bqmodel:is	Enzyme Nomenclature	<input type="text"/> Add Home

Reactions (7) ⌵ ⌶ ⌷

creation of cyclin ⊞
 Reactants:
 Products: [Cyclin](#)
 Modifiers:

bqbiol:isVersionOf	set #1	Gene Ontology translation Remove
Update	Enzyme Nomenclature	<input type="text"/> Add Home
bqmodel:is	Enzyme Nomenclature	<input type="text"/> Add Home

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BioModels Version 3

Relational Database

- **Xindice has file size limitation -> OutOfMemoryError**
- **MySQL5.1 supports XML functions**
- **Create indexes for SBML**

Acknowledgments

EBI

- Nicolas Le Novère
- Marco Donizelli
- Lu Li
- Nicolas Rodriguez
- Mélanie Courtot
- Arnaud Henry
- Camille Laibe
- Enuo He

SBML Team

- Michael Hucka
- Sarah Keating
- Harish Dharuri
- Benjamin J. Bornstein

BioModels Database is funded by:



European Molecular
Biology Laboratory



National Institute of
General Medical Sciences