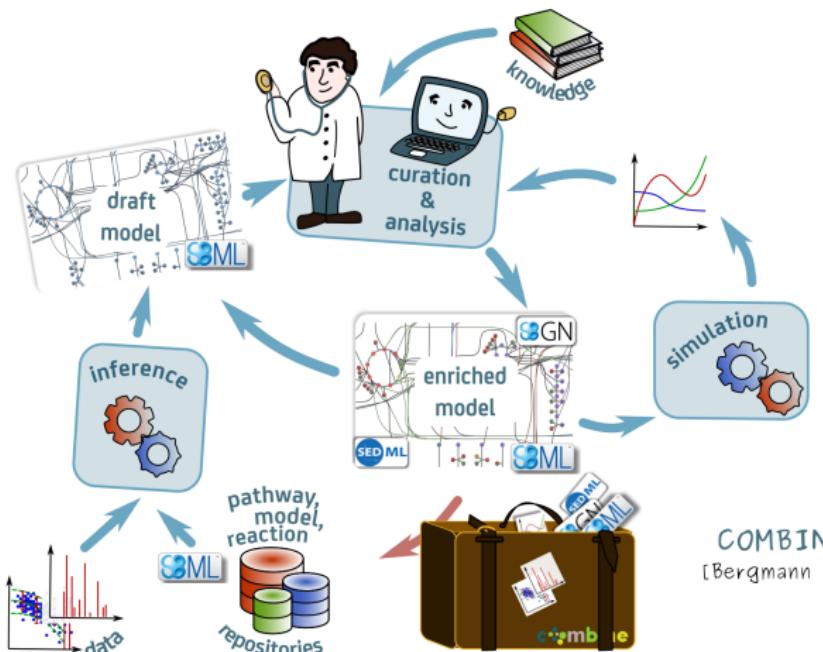


# A MODELING WORKFLOW IN SYSTEMS BIOLOGY: OVERVIEW

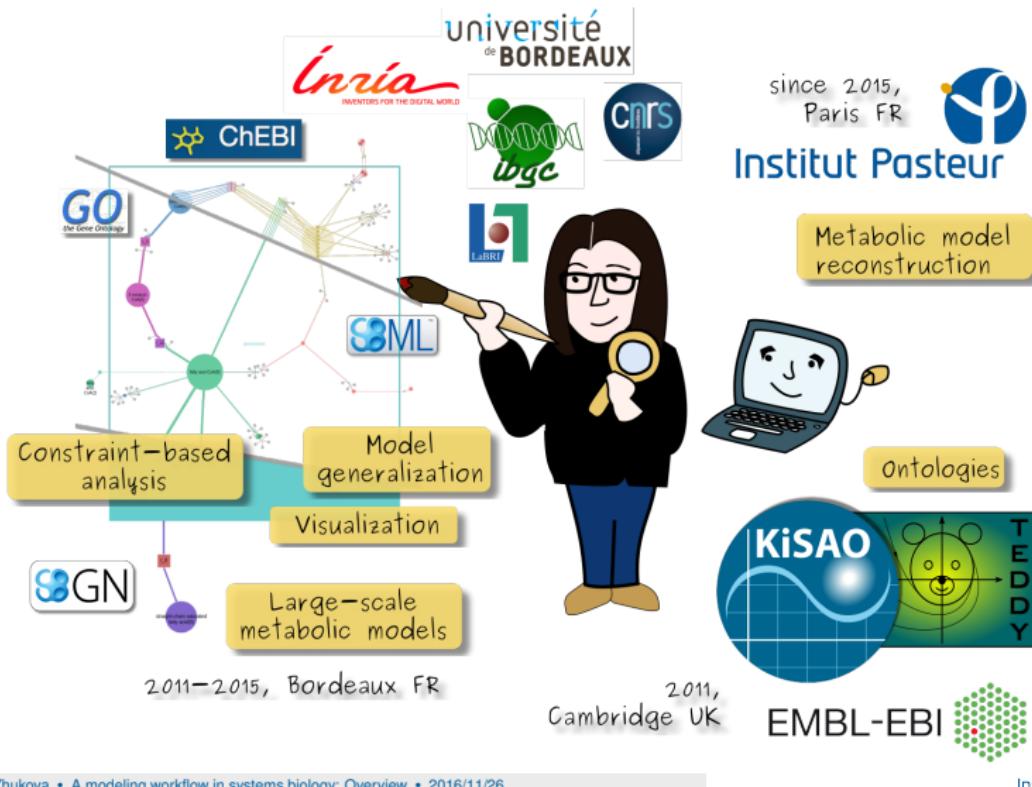
- Anna Zhukova
- 2016/11/26

# Modeling workflow

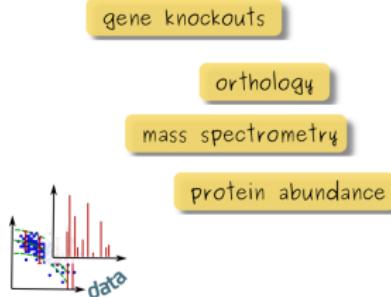


COMBINE archive  
[Bergmann et al., 2014]

# Who am I?



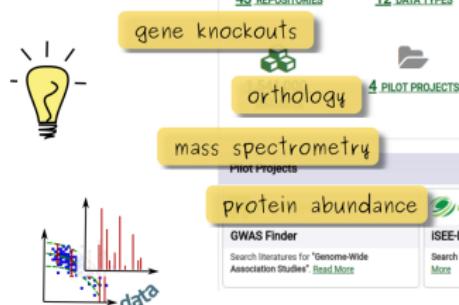
# Modeling workflow



# Modeling workflow

Findability  
Accessibility  
Interoperability  
Reusability

[Wilkinson et al., 2016]



<https://datamed.org> biomedical and healthCare Data Discovery Index Ecosystem **bioCADDIE**

About Feedback+ Submit Login

Engaging The Community Toward a Data Discovery Index (v1.5)

Search for data through bioCADDIE

Search for data set Search for repository Advanced Search help

Statistics

43 REPOSITORIES

12 DATA TYPES

Top 8 Repositories

Repository	Number of Datasets
UniProt	438182
GDC	262293
ClinVar	204689
ClinicalTrials	200674
BioProject	155850
PDB	122339
Dryad	82837
ArrayExpress	68189

New Features

Nov 23, 2016. v1.5

- Increased coverage to twice the number of repositories
- Total number of datasets doubled
- Repositories mapped to DATS 2.1 metadata model
- Sorting on publication date of the dataset
- Visualization of results via timeline
- Usability enhancements based on user feedback and user interviews
- User-reported issues resolved

Jun 30, 2016. v1.0

- Filter results by accessibility and authorization
- Synonym expansion using ontologies ...

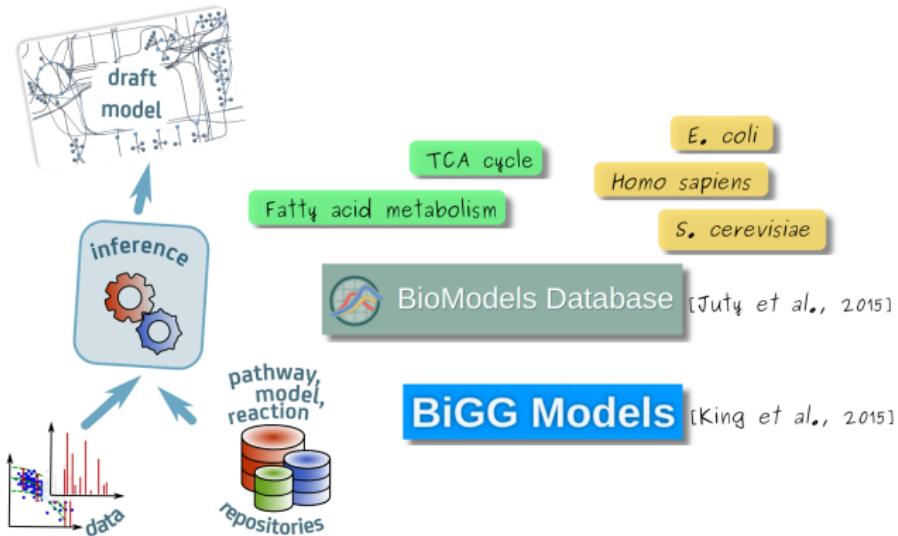
GWAS Finder

ISEE-DELVE

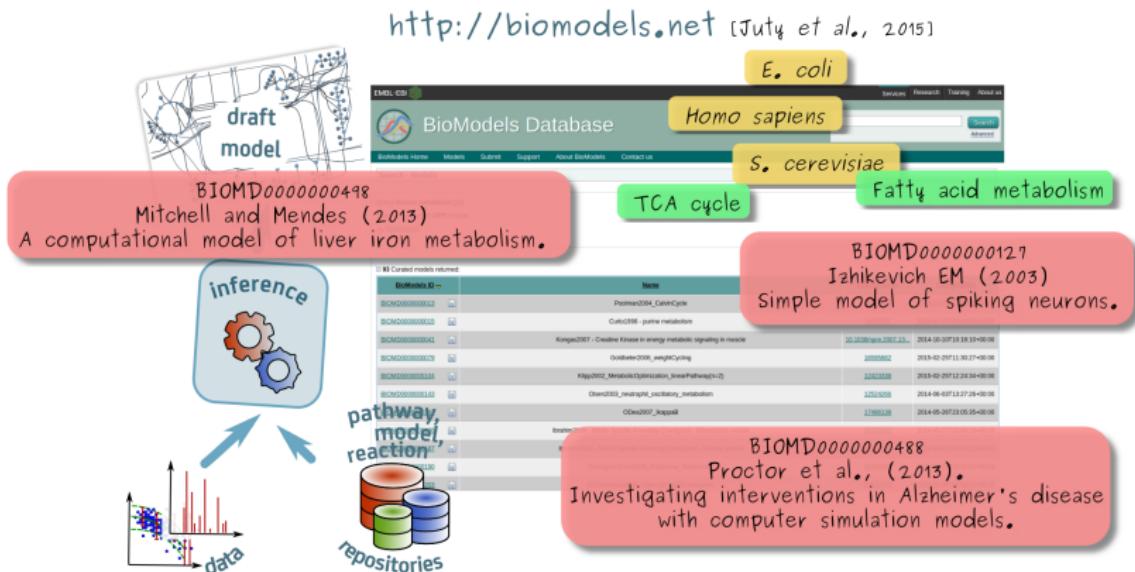
DataRank

Data Citation Discovery

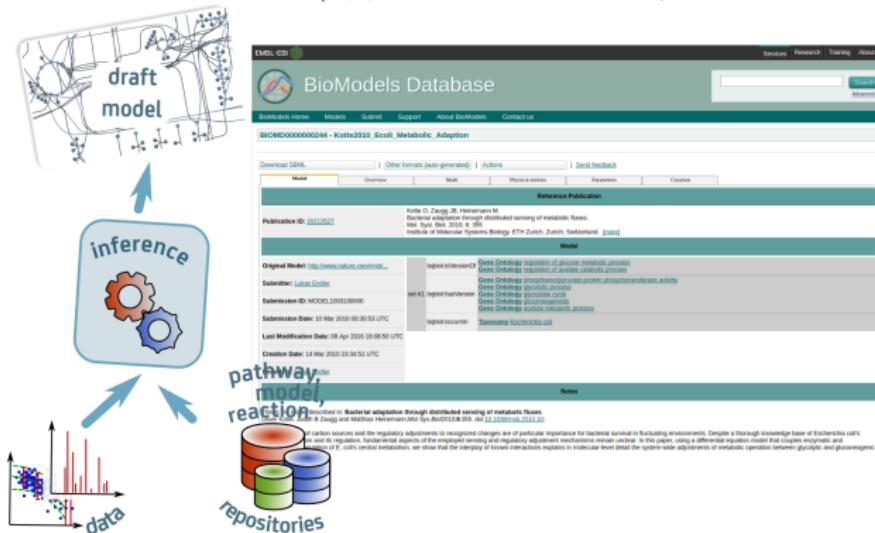
# Modeling workflow



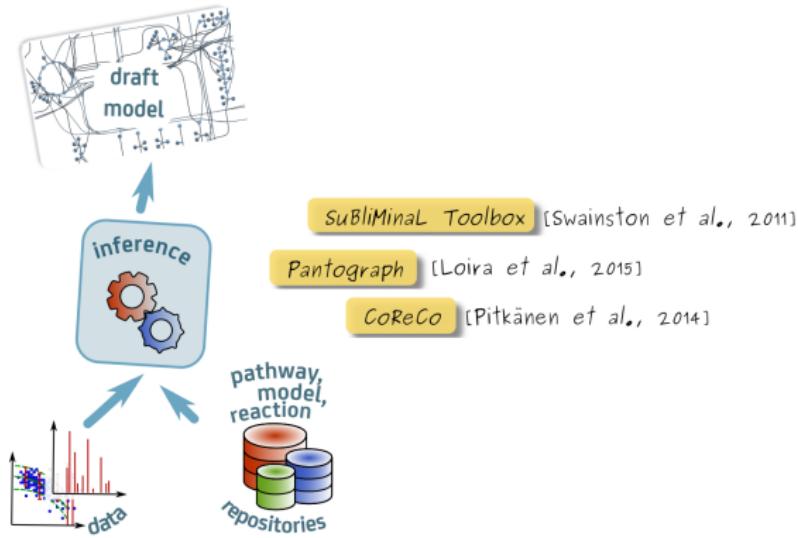
# Modeling workflow



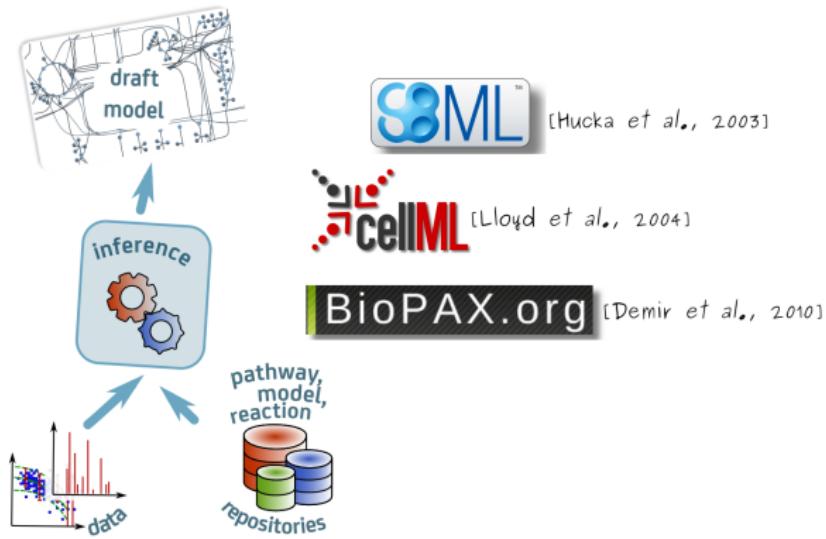
# Modeling workflow



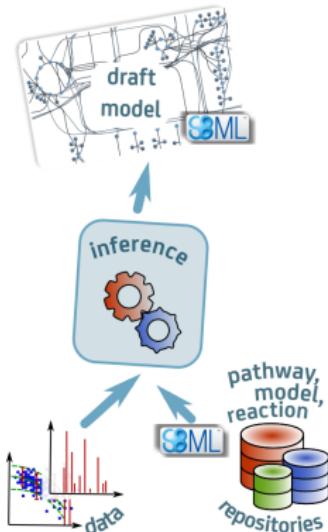
# Modeling workflow



# Modeling workflow



# Modeling workflow

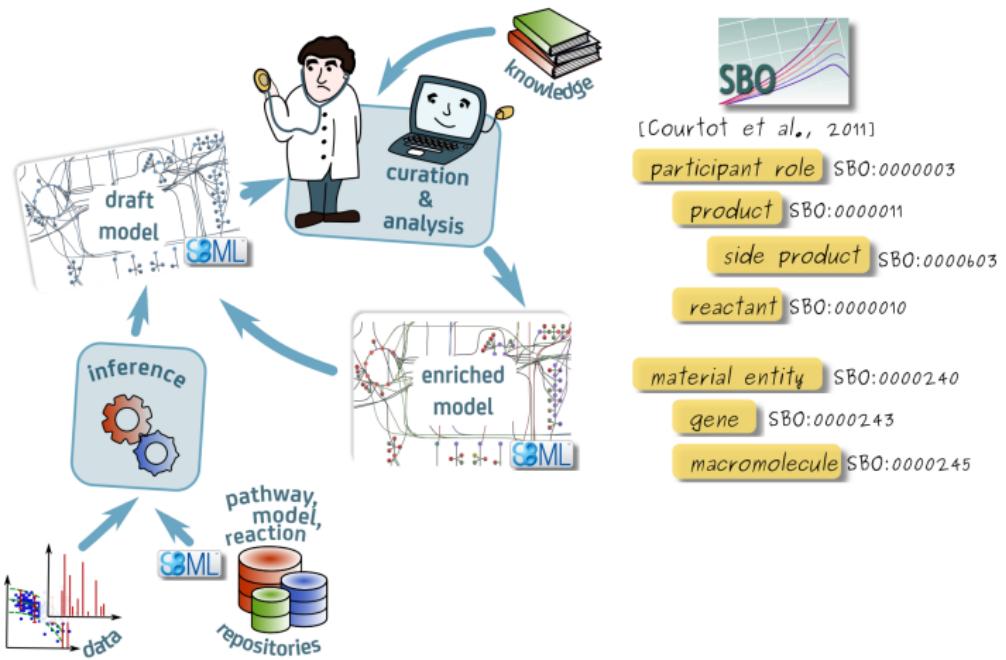


<http://sbml.org> [Hucka et al., 2003]

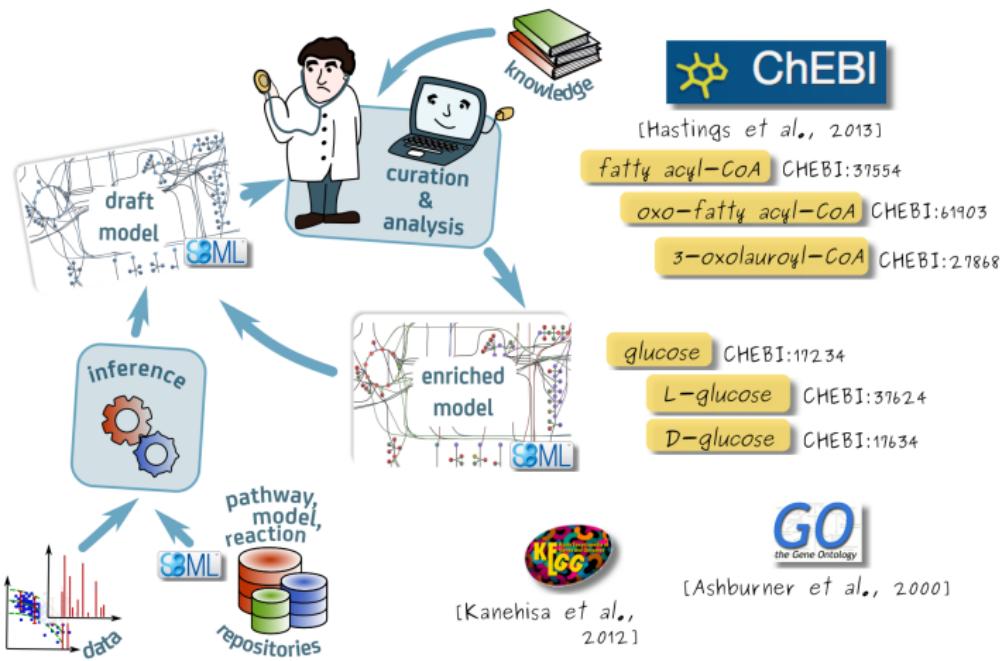
```
<sbml xmlns:rdf=...> <model metaid="meta_ymn" id="ymn">
  <listOfCompartments>
    <compartment id="c_03" name="cytoplasm" .../>
  ...
  <listOfSpecies>
    <species id="s_0803" name="H2O" compartment="c_03" ...>
      <annotation> ...
        <rdf:li rdf:resource=".../CHEBI:15377"/>
      ...
    </species>
  ...
  <listOfReactions>
    <reaction id="r_0138" name="adenine deaminase"
      rev...="true"...>
      <listOfReactants>
        <speciesRef... species="s_0803" stoichiometry="1" .../>
        ...
      </listOfReactants>
      <listOfProducts>
        <speciesRef... species="s_0419" stoichiometry="1" .../>
        <speciesRef... species="s_0843" stoichiometry="1" .../>
      </listOfProducts>
    </reaction>
  ...
</sbml>
```

libSBML [Bornstein et al., 2008]

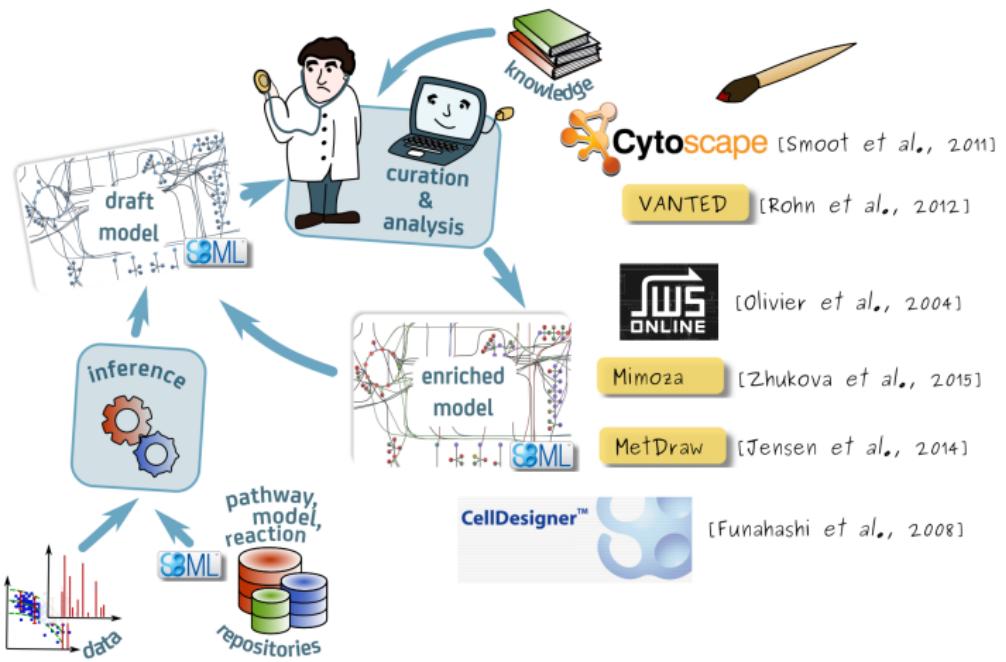
# Modeling workflow



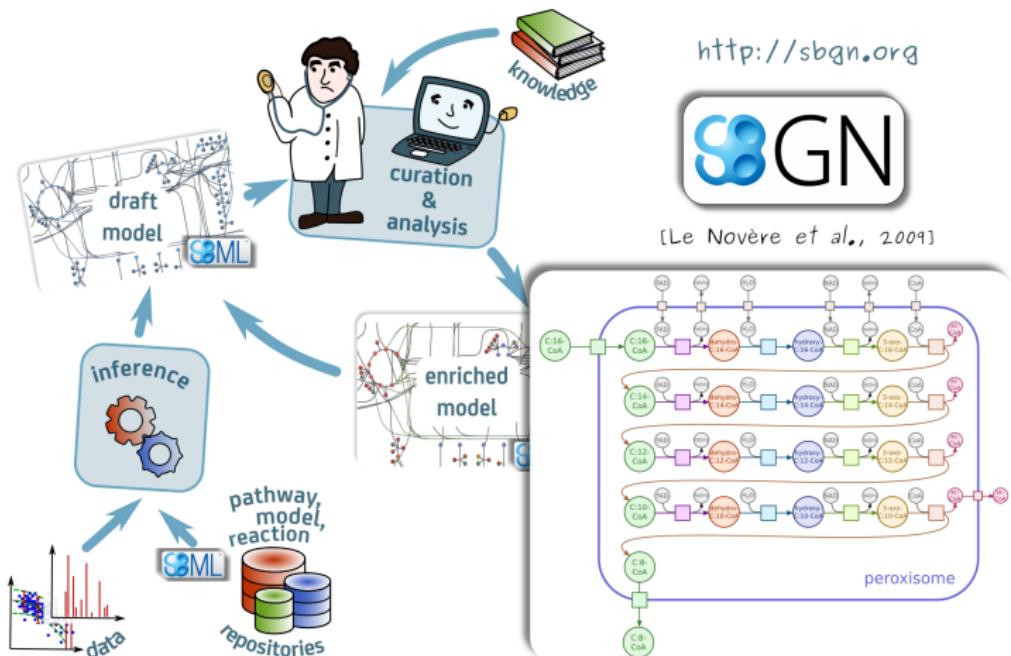
# Modeling workflow



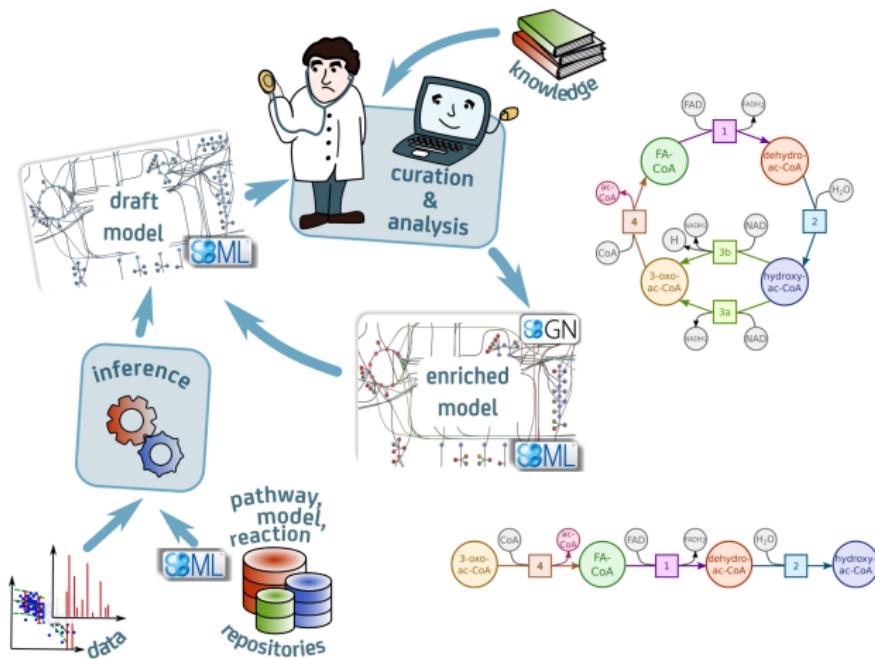
# Modeling workflow



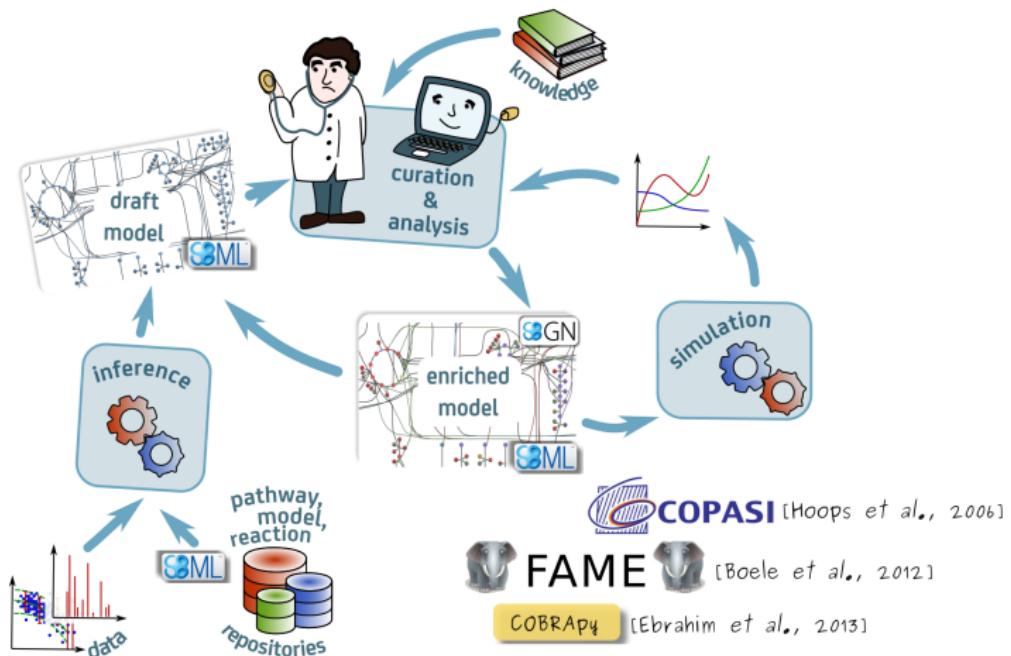
# Modeling workflow



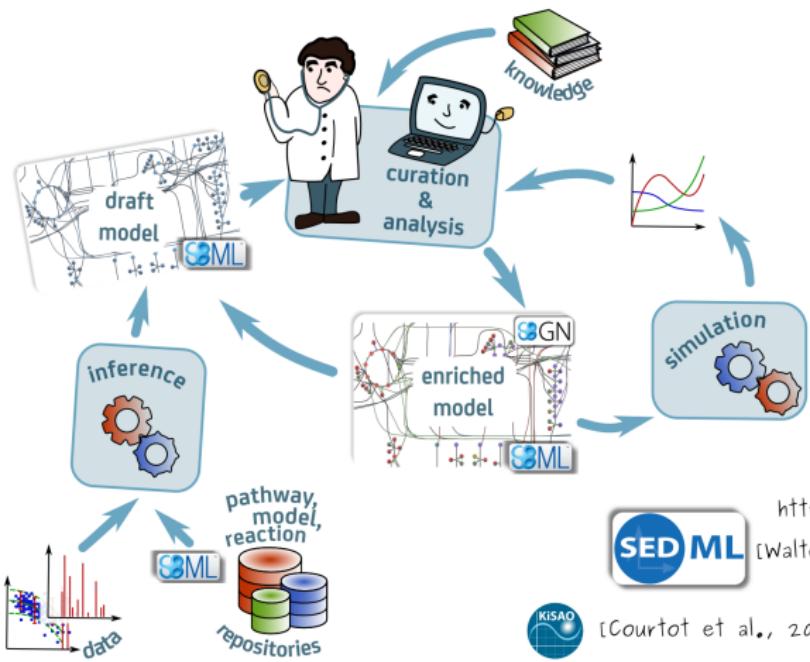
# Modeling workflow



# Modeling workflow



# Modeling workflow



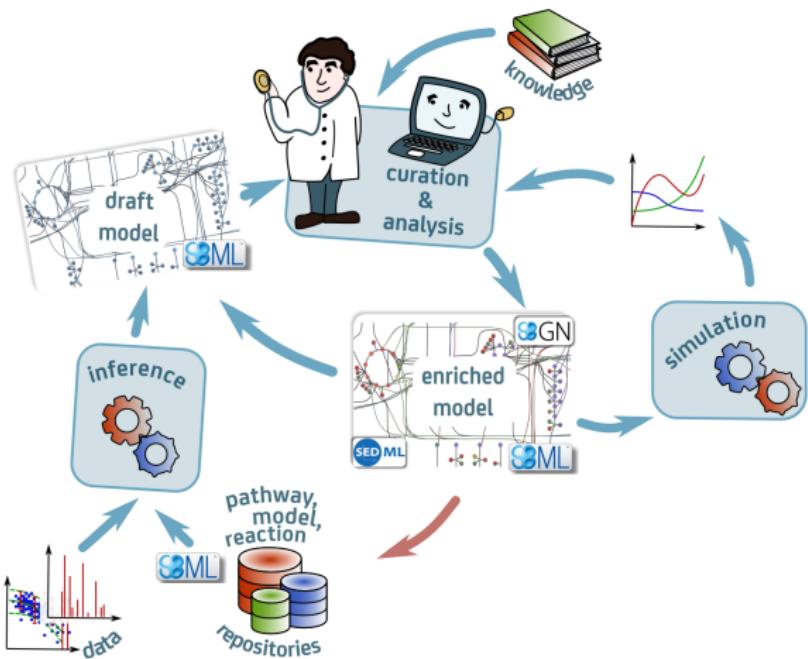
<http://sedml.org>  
[Walters et al., 2011]



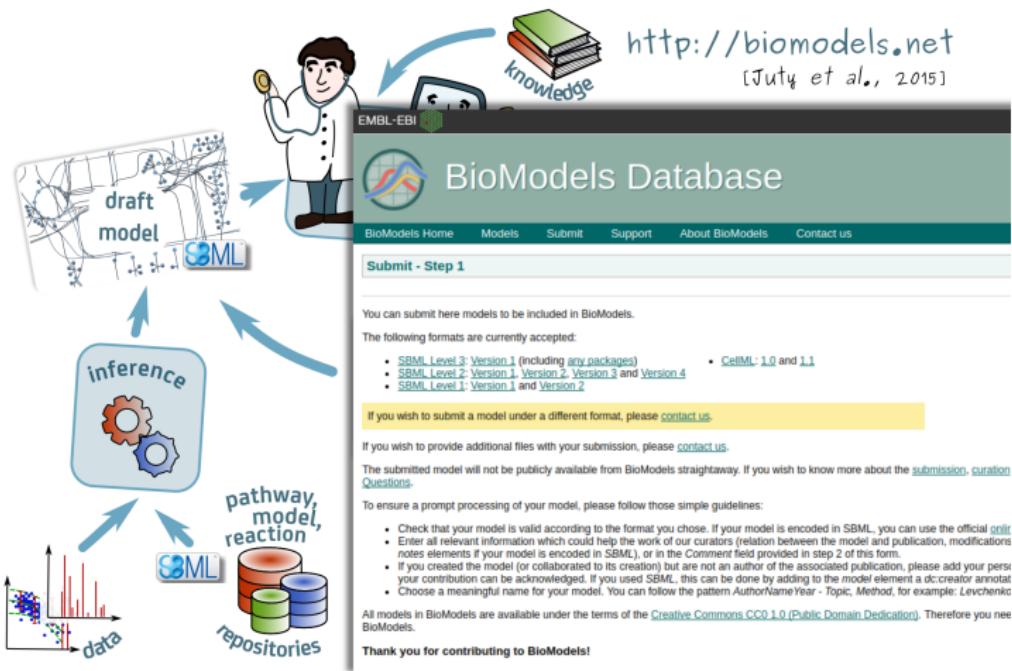
[Courtot et al., 2011]



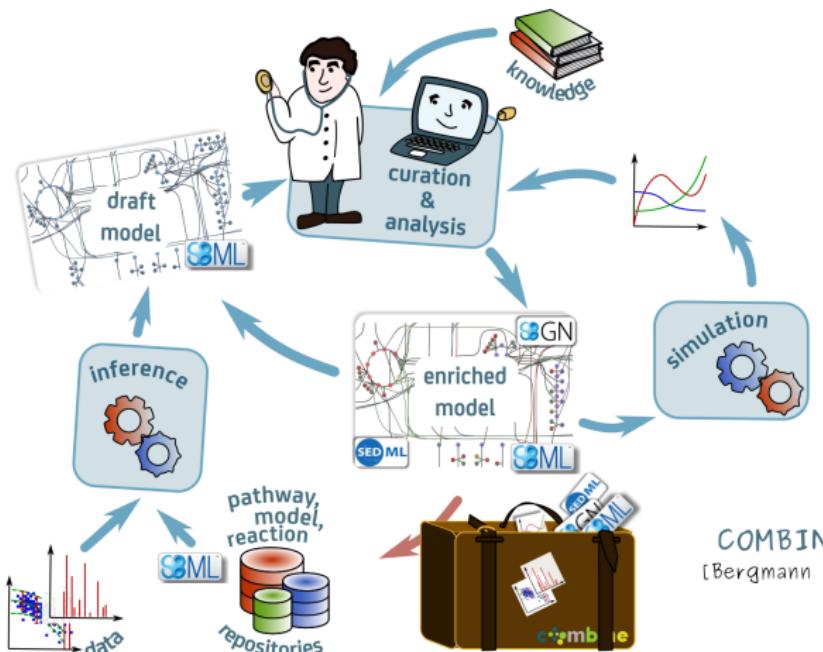
# Modeling workflow



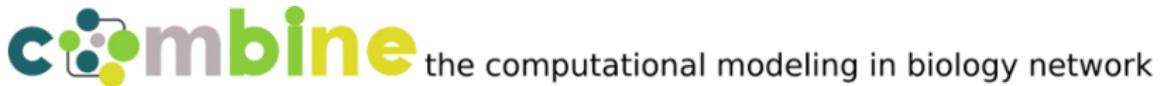
# Modeling workflow



# Modeling workflow



All those standards and more: <http://co.mbine.org>



COMBINE 2016   Standards   Events   Documents   About   Forums    Search

#### COMBINE

- Home
- Help
- Sign-in

#### Coordinating standards for modeling in biology

The 'C'OMputational Modeling in Biology' NEtwork (COMBINE) is an initiative to coordinate the development of the various community [standards and formats](#) for computational models. By doing so, it is expected that the federated projects will develop a set of interoperable and non-overlapping standards covering all aspects of modeling in biology.

Building on the experience of mature projects, which already have stable specifications, software support, user-base and community governance, COMBINE will help foster or support fledgling efforts aimed at filling gaps or new needs. As those efforts mature, they may become part of the [core set of COMBINE standards](#).

One of the initial activities of COMBINE is to coordinate the organization of scientific and technical [events](#) common to several standards. Those events, as others related to our field of research are [gathered in a calendar](#).

To receive announcements from COMBINE, subscribe to the twitter [COMBINE news](#)

To discuss the goals, organization and operation of COMBINE, subscribe to [COMBINE discuss](#).

To report issues about the co.mbine.org website, send a mail to [combine-support @ googlegroups.com](mailto:combine-support@googlegroups.com)

#### Tweets by [@combine\\_coord](#)

COMBINE Retweeted



# More ontologies?

<http://bioportal.bioontology.org> [Noy *et al.*, 2009]

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Welcome to BioPortal, the world's most comprehensive repository of biomedical ontologies. Current Release: 4.29 (October 2016)

For help using BioPortal, click on this icon:

Search all ontologies    Find an ontology    Search resources

Advanced Search    Explore    Search

Ontology Visits (October 2016)

Current Procedural Terminology (CPT)	47529
Medical Dictionary for Regulatory Activities (MEDDRA)	18973
RxNORM (RXNORM)	14577
Systematized Nomenclature of Medicine - Clinical Terms (SNOMEDCT)	10038
National Drug Data File (NDDF)	6573

Latest Notes

What is measured is carbon isotope composition (Plant Trait Ontology)  
7 months ago by BrenOli  
I would suggest that there should be subcategories for "Carbon Isotope Discrimination", as what ...

New Relationship Proposal: certiMorgan is by definition dimensionless (Units of Measurement Ontology)  
10 months ago by grimaldi

TCA cyc  
Citrate cycle (TCA cycle) 0 from: Pathway Terminology System  
Citrate Cycle (TCA Cycle) Pathway 0 from: National Cancer Institute Thesaurus  
Citric acid cycle (TCA cycle) 0 from: Human Interaction Network Ontology  
Alzheimer's disease (CRISP) => CDK5 (ADO)  
REST Mapping 10/24/2016 by SAM-PETERS  
CDK5 (ADO) => Alzheimer's disease (CRISP)  
REST Mapping 10/24/2016 by SAM-PETERS  
Malnutrition (MEDLINEPLUS) => Malnutrition (NCIT)  
REST Mapping 09/29/2016 by Anagruz  
Malnutrition (NCIT) => Malnutrition (MEDLINEPLUS)  
REST Mapping 09/29/2016 by Anagruz

# More ontologies?

<http://www.obofoundry.org> [Smith *et al.*, 2007]



About ▾   Principles ▾   Ontologies ▾   Citation ▾   Participate ▾   FAQ ▾   Legacy ▾   Search Ontobee   Submit

## The OBO Foundry

The OBO Foundry is a collective of ontology developers that are committed to collaboration and adherence to shared principles. The mission of the OBO Foundry is to develop a family of interoperable ontologies that are both logically well-formed and scientifically accurate. To achieve this, OBO Foundry participants voluntarily adhere to and contribute to the development of an evolving set of principles including open use, collaborative development, non-overlapping and strictly-scoped content, and common syntax and relations, based on ontology models that work well, such as the Gene Ontology (GO).

The OBO Foundry is overseen by an Operations Committee with Editorial, Technical and Outreach working groups. The processes of the Editorial working group are modelled on the journal refereeing process. A complete treatment of the OBO Foundry is given in "The OBO Foundry: coordinated evolution of ontologies to support biomedical data integration".

On this site you will find a table of ontologies, available in several formats, with details for each, and documentation on OBO Principles.

You can contribute to this site using GitHub [OBOFoundry/OBOFoundry.github.io](https://github.com/OBOFoundry/OBOFoundry.github.io) or get in touch with us at [obo-discuss@sourceforge.net](mailto:obo-discuss@sourceforge.net).

Download table as: [[YAML](#) | [JSON-LD](#) | [RDF/Turtle](#)]

chebi	Chemical Entities of Biological Interest	A structured classification of molecular entities of biological interest focusing on 'small' chemical compounds. <a href="#">Detail</a>								
doid	Human Disease Ontology	An ontology for describing the classification of human diseases organized by etiology. <a href="#">Detail</a>								
go	Gene Ontology	An ontology for describing the function of genes and gene products <a href="#">Detail</a>								

# All together: <https://biosharing.org>

The screenshot shows the homepage of biosharing.org. At the top, there's a navigation bar with links for Standards, Databases, Policies, Collections, Add/Claim Content, and Stats. Below the header, there are three main sections: 'Find' (Recommendations), 'Discover' (Collections), and 'Learn' (Educational). The 'Find' section shows a search bar with 'kisao' typed in, and checkboxes for Standards, Databases, Policies, and Collections/Recommendations. It also includes a 'Search' button and an 'Advanced Search' link. The 'Discover' section features a 'Collections' icon and a description of standards grouped by domain or species. The 'Learn' section has an 'Educational' icon and a brief description about standards and their use. Below these sections, there are three large cards: '670 Standards' (with icons for artifact, model/format, and reporting guideline), '827 Databases' (with icons for protein, genome, and DNA), and '85 Policies' (with icons for funder, journal, and society). Each card has a 'View all' button at the bottom.

**Find**

**Discover**

**Learn**

**Recommendations**  
Standards and/or databases recommended by journal or funder data policies.

**Collections**  
Standards and/or databases grouped by domain, species or organization.

**Educational**  
About standards, their use in databases and policies, and how you can help you.

**Search**

**Advanced Search**

**Search Wizard**

**kisao**

Standards    Databases    Policies    Collections/Recommendations

**670 Standards**

Terminology Artifact  
Model/Format  
Reporting Guideline

View all

**827 Databases**

Protein  
Genome  
DNA

View all

**85 Policies**

Funder  
Journal  
Society

View all

# Wishing you a pleasant modeling flight!



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foundation with official  
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