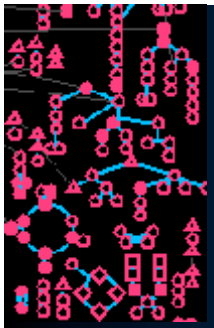


Databases and Algorithms for Pathway Bioinformatics

Peter D. Karp, Ph.D.

Bioinformatics Research Group

SRI International

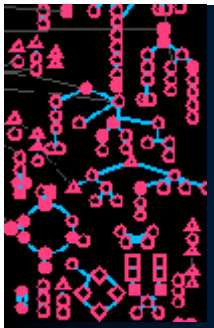
pkarp@ai.sri.com

BioCyc.org

EcoCyc.org

MetaCyc.org

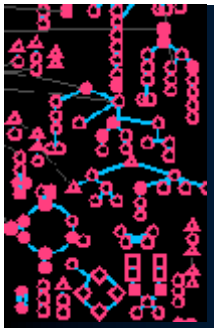
HumanCyc.org



MOD Home Pages

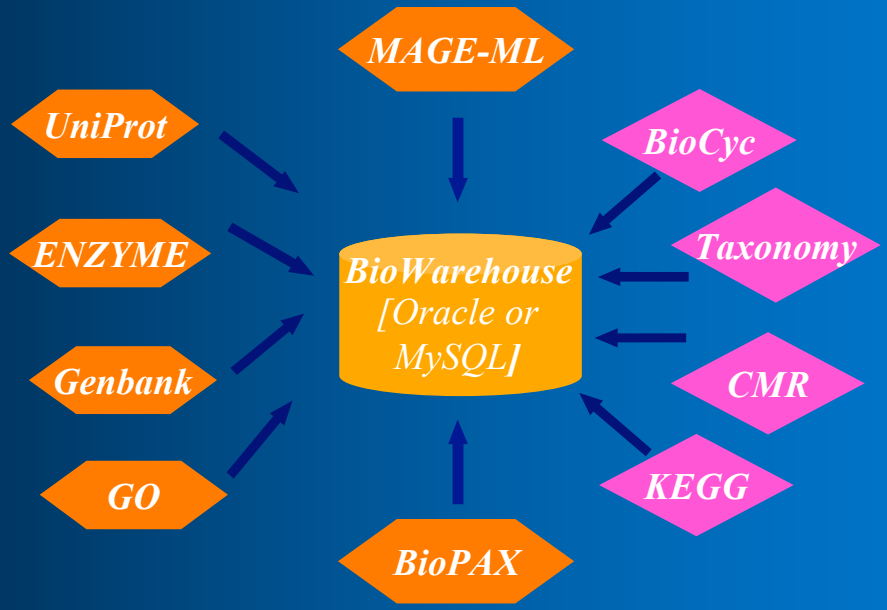
- **Learn or standardize?**

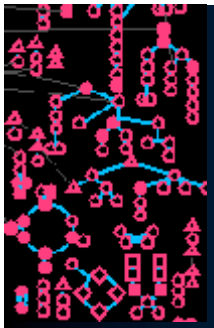
- **Top / Left**
- **Cascading menus or not**
- **Must-haves on home page:**
  - Citing MOD
  - Software/data download
  - Contact us
  - News
  - Publications
  - Statistics
  - Update history
  - Credits



BioWarehouse

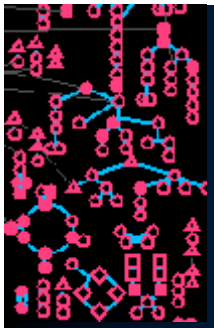
Peter D. Karp, Tom J. Lee,
Valerie Wagner, Yannick Pouliot





Motivations

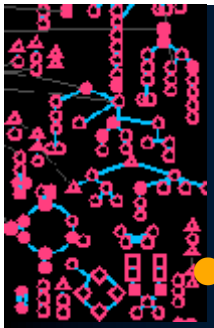
- Hundreds of bioinformatics DBs exist
- Important problems involve queries across multiple DBs



Why is the Multidatabase Approach Alone Not Sufficient?

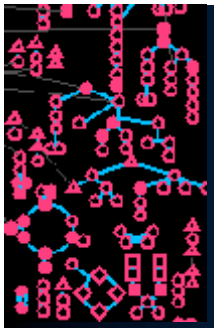
- Multidatabase query approaches assume databases are in a queryable DBMS
- Most sites that do operate DBMSs do not allow remote query access because of security and loading concerns
- Users want to control data stability
- Users want to control speed of their hardware
- Internet bandwidth limits query throughput
- Users need to capture, integrate and publish locally produced data of different types

- Multidatabase and Warehouse approaches complementary



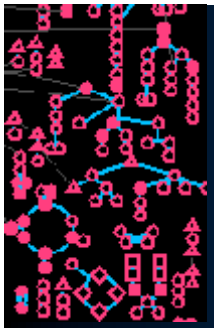
Technical Approach

- **Multi-platform support: Oracle (10g) and MySQL**
- **Schema support for multitude of bioinformatics datatypes**
- **Create loaders for public bioinformatics DBs**
  - Parse file format of the source DB
  - Semantic transformations
  - Insert DB contents into warehouse tables
- **Provide Warehouse query access mechanisms**
  - SQL queries via ODBC, JDBC, OAA
- **Operate public BioWarehouse server: publichouse**



BioWarehouse Schema

- **Manages many bioinformatics datatypes simultaneously**
  - Pathways, Reactions, Chemicals
  - Proteins, Genes, Replicons
  - Sequences, Sequence Features
  - Organisms, Taxonomic relationships
  - Computations (sequence matches)
  - Citations, Controlled vocabularies
  - Links to external databases
- **Each type of warehouse object implemented through one or more relational tables (currently 43)**



Warehouse Schema

- **Different databases storing the same biological datatypes are coerced into same warehouse tables**
- **Design of most datatypes inspired by multiple databases**
- **Representational tricks to decrease schema bloat**
  - Single space of primary keys
  - Single set of satellite tables such as for synonyms, citations, comments, etc.

BioWarehouse Loaders

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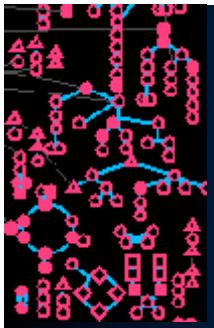
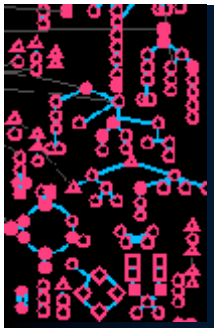
Database	Loader Language	Input Format	Comments
Any BioPAX	Java	BioPAX	Protein interaction data only
BioCyc	C	BioCyc attribute-value	Pathway/Genome Databases
CMR	C	CMR column-delimited	Comprehensive Microbial Resource: 150+ microbial genomes
ENZYME	Java	ENZYME attribute-value	Enzyme Commission set of reactions
Genbank	Java	XML derived from ASN.1	Bacterial subset of Genbank
Gene Ontology	Java	OBO XML	Hierarchical controlled vocabulary
KEGG	C	KEGG format	Metabolic pathway data
Any MAGE-ML	Java	MAGE-ML format	Microarray gene expression data
NCBI Taxonomy	C	Taxonomy format	Organism taxonomy
UniProt	Java	UniProt XML	SWISS-PROT and TrEMBL

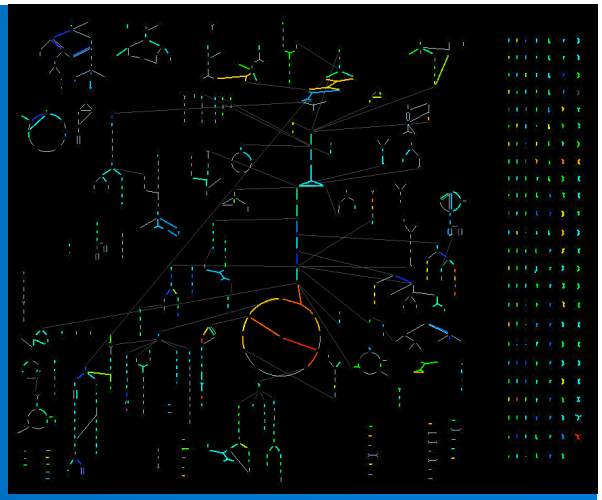


Uses of BioWarehouse

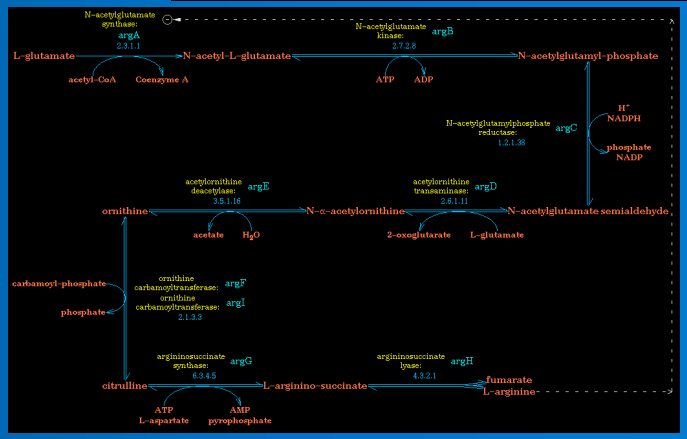
- **SRI Bioinformatics Research Group**
  - Extract genome data from CMR for generation of BioCyc Tier 3
  - Use CMR for genome-context extensions to pathway hole filler
  - Enzyme genomics research

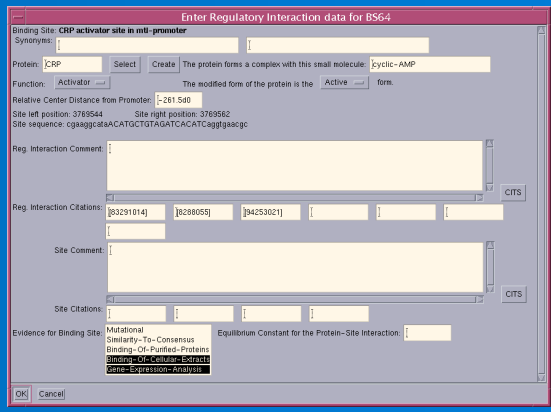


Pathway Tools Software



- **PathoLogic**
  - Predicts operons, metabolic network, pathway hole fillers, from genome
  - Computational creation of new model organism databases
  - Can work as complete MOD system, or pathway module only

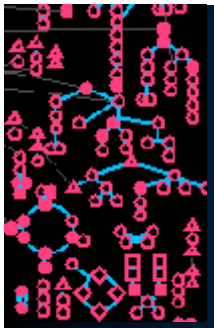




- **Pathway/Genome Editors**
  - Distributed curation of PGDBs
  - Distributed object database system, interactive editing tools

- **Pathway/Genome Navigator**
  - WWW publishing of PGDBs
  - Querying, visualization of pathways, chromosomes, operons
  - Pathway visualization of omics data
  - Global comparisons of metabolic networks

Brg.ai.sri.com/ptools/



Pathway Tools Update

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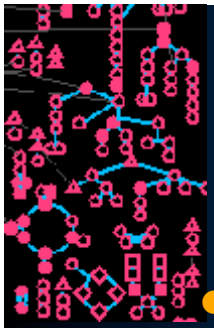
- Version 10.5
- Ontology upgrade for signaling interactions
- Consistency checker
- Generate metabolic map poster
- Zooming in Overview
- Sequence retrieval tool
- BioPAX export, pathway page
- New reaction editor
- Spelling checker

- Version 11.0
- Regulatory network viewer



Acknowledgements

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