LINKINGOPENDATA
W3C SWEO Community Project

ENABLING TAILORED THERAPEUTICS WITH LINKED DATA

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Linking Open Drug Data (LODD) Task Froce
http://esw.w3.org/topic/HCLSIG/LODD

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Presentation at the Linked Data On the Web (LDOW) 2009 Workshop

Outline

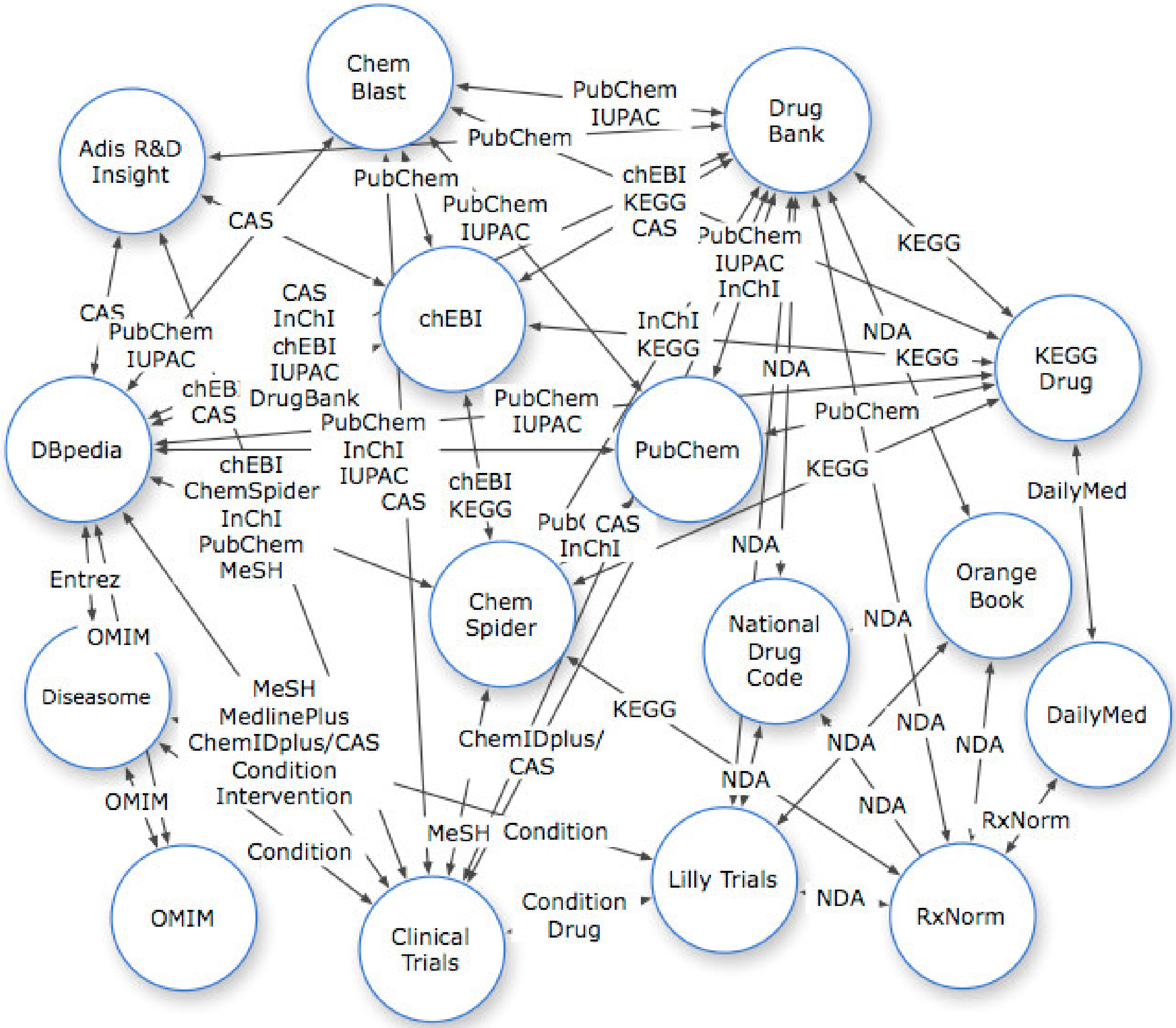
- Linking Open Drug Data Project
  - Objectives and Status
- Published linked data sources
- Interlinking of the data sources
- Business use cases
- Conclusion and Future Work

Linking Open Drug Data

- An HCLSIG task force
  - Started October 1st, 2008
- Primary Objectives
  - Survey publicly available data sets about drugs
  - Publish and interlink these data sets on the Web
  - Explore interesting questions that could be answered if the data sets are linked

Survey of Existing Data sets

- □ http://esw.w3.org/topic/HCLSIG/LODD/Data



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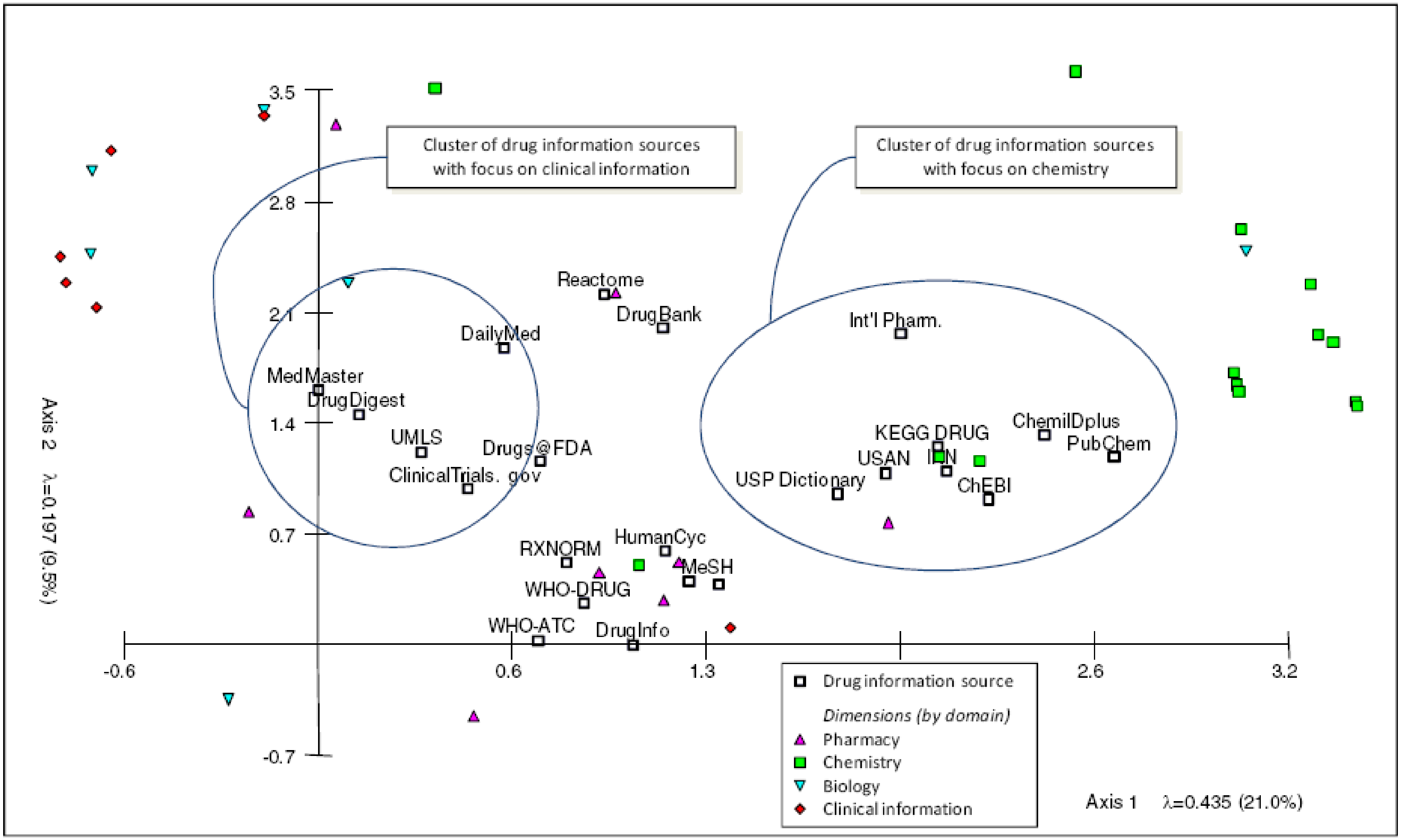
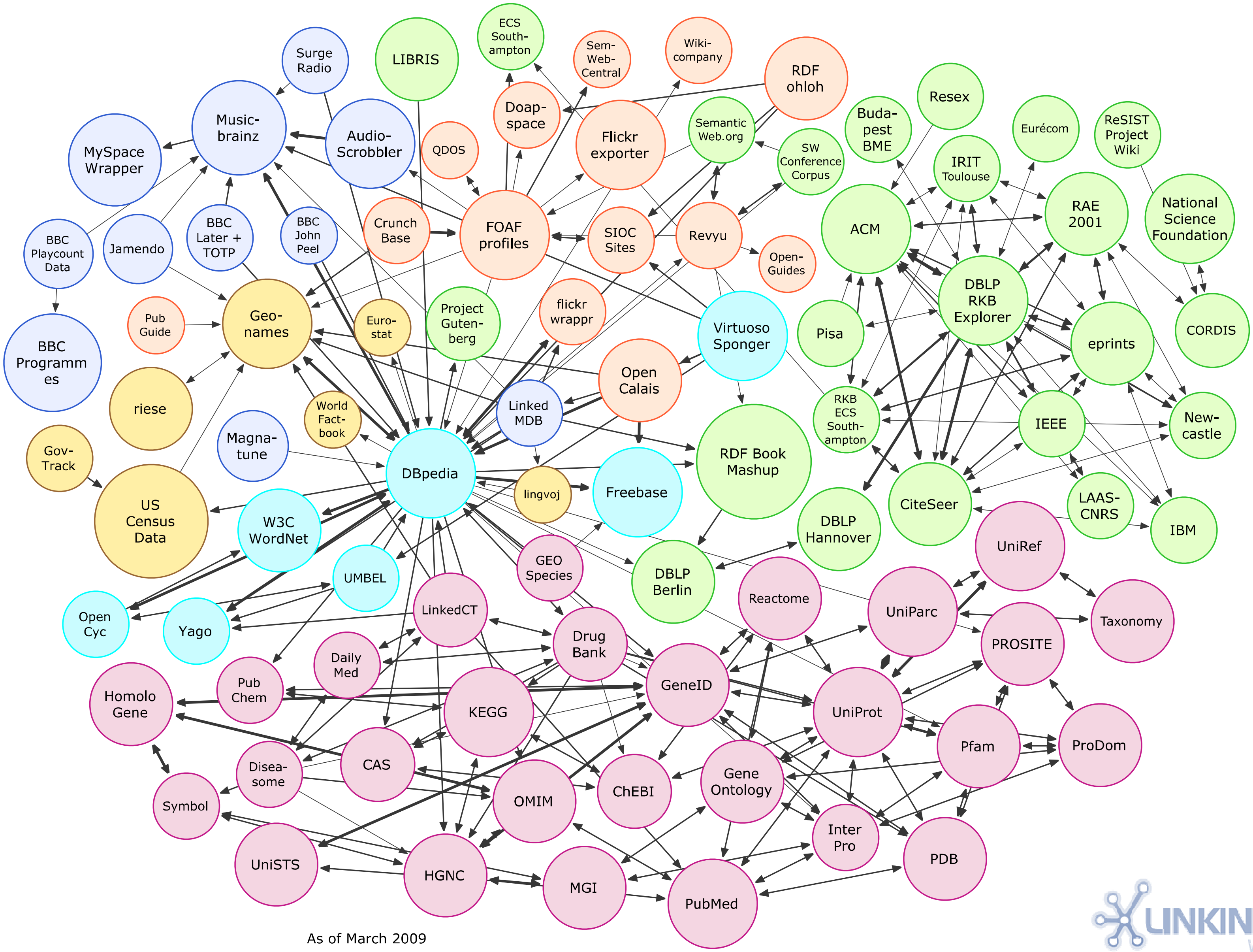
Drug Data Sources



- Source: Mark Sharp, et al. (AMIA 2008)
  A Framework for Characterizing Drug Information Sources

Extending LOD cloud



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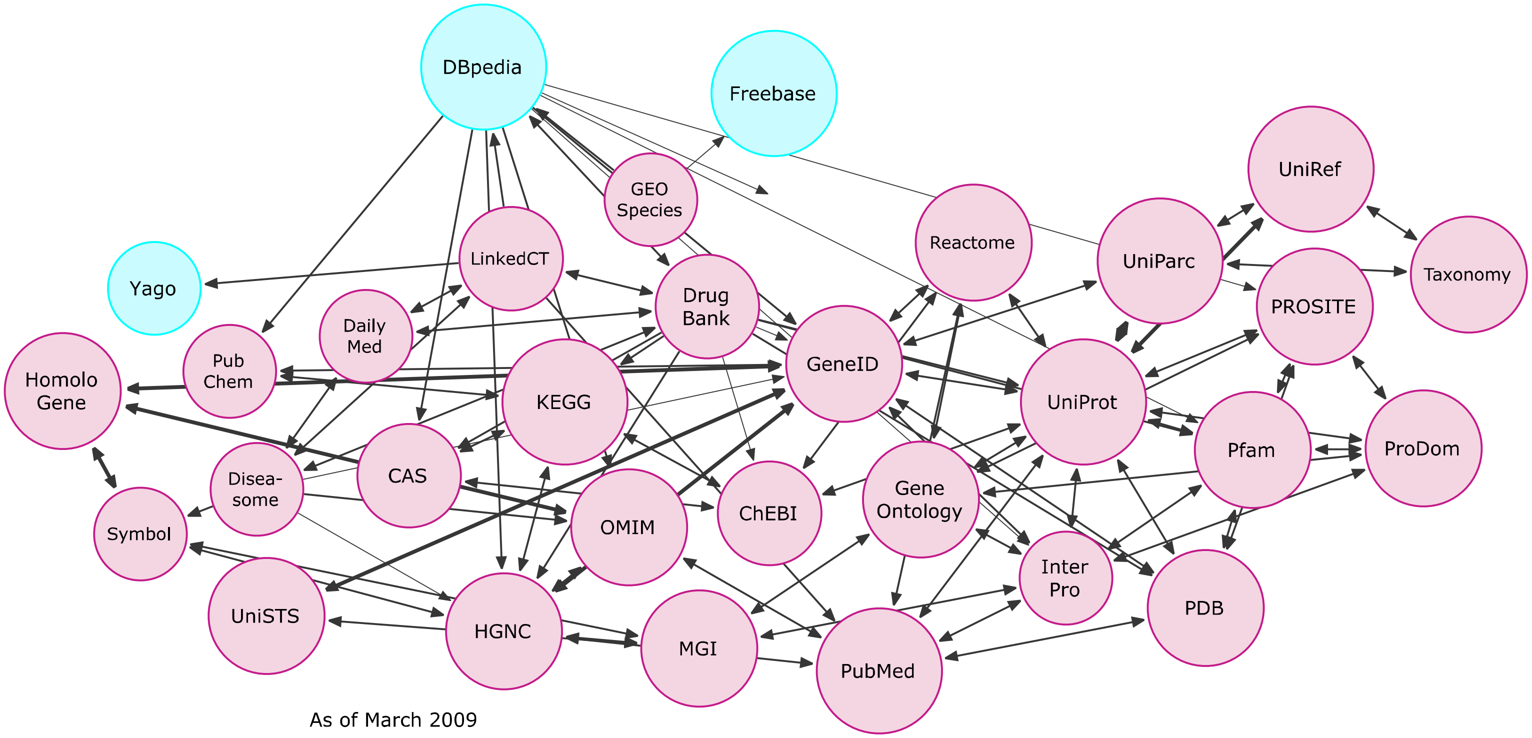
HCLS in LOD cloud



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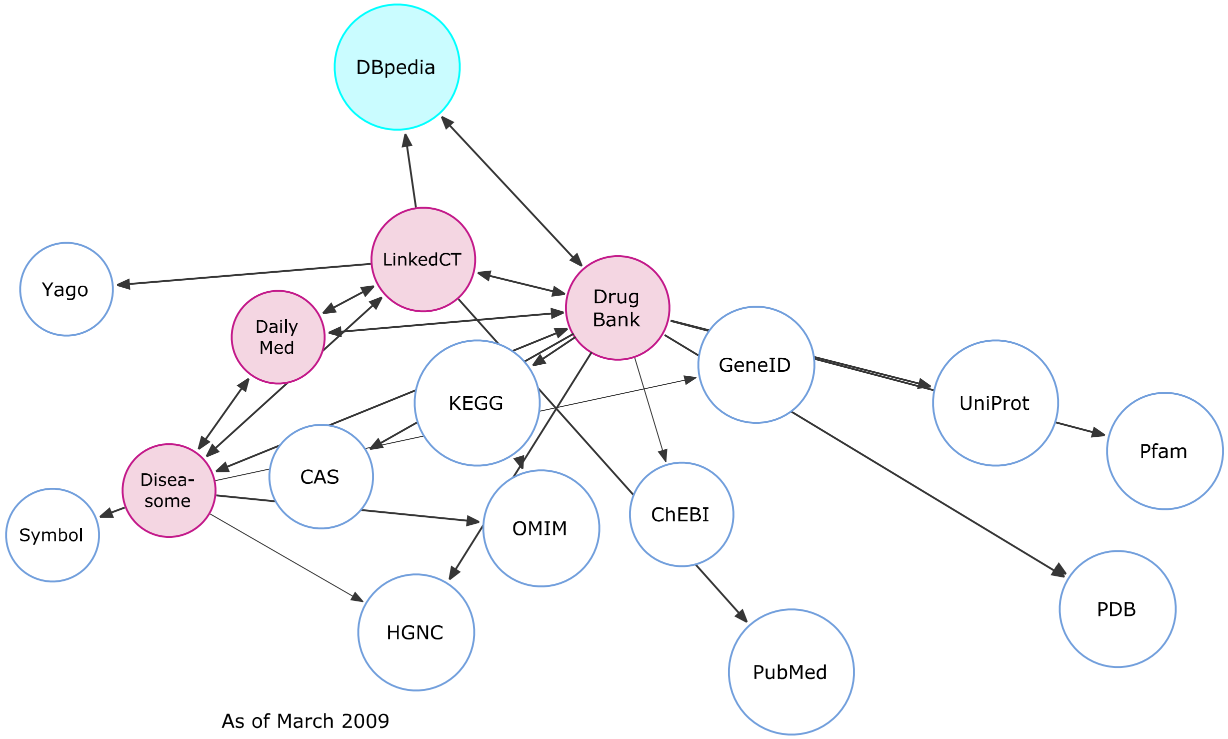
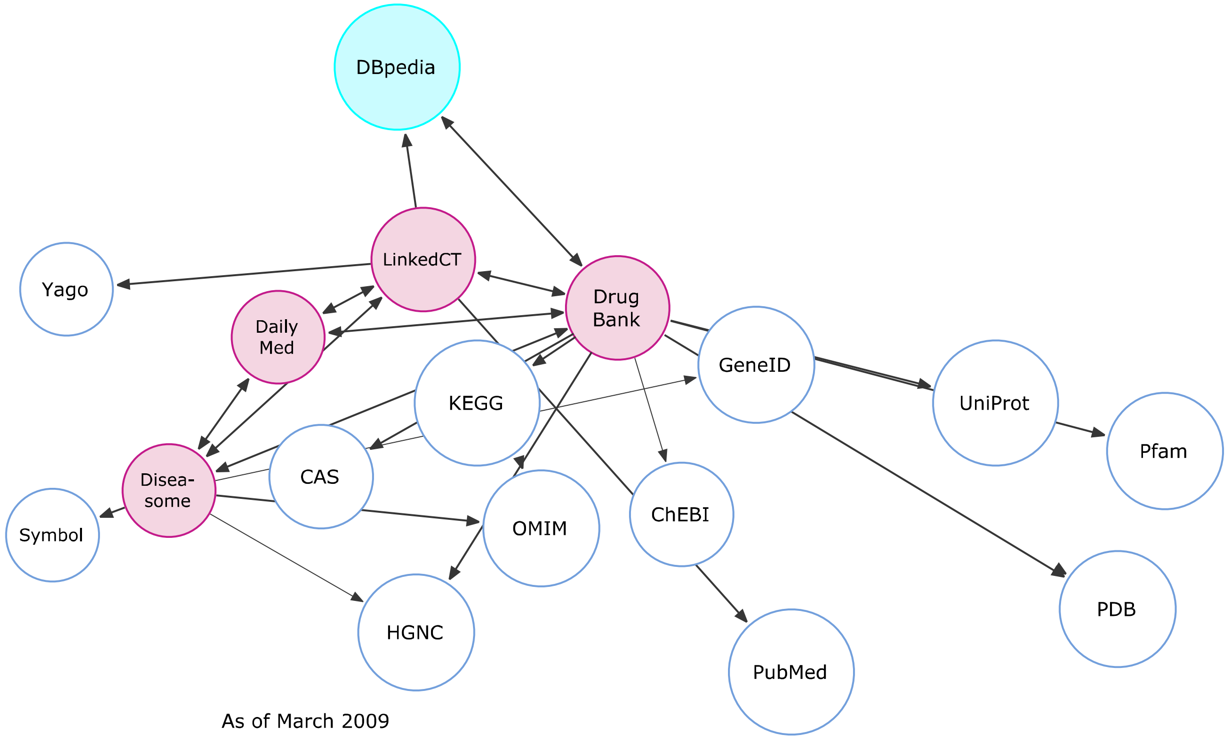
LODD in LOD cloud



As of March 2009

- Published Data Sets
  - LinkedCT
  - Diseasome
  - DailyMed
  - DrugBank

LODD in LOD cloud



As of March 2009

- Interlinked to:
  - DBpedia/YAGO
  - Symbol
  - CAS
  - HGNC
  - KEGG
  - OMIM
  - ChEBI
  - GeneID
  - PubMed
  - UniProt
  - Pfam
  - PDB

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Published Datasets

- LinkedCT

  http://linkedct.org

  - From ClinicalTrials.gov
    - Online registry of clinical trials conducted in the United States and around the world
    - Published in XML
  - More than 60,000 trials
  - 7,011,000 triples
- DrugBank

  http://www4.wiwiss.fu-berlin.de/drugbank/

  - A repository of almost 5000 FDA-approved small molecule and biotech drugs
    - Published as DrugBank DrugCards
  - 1,153,000 triples

Published Datasets

- DailyMed

  http://www4.wiwiss.fu-berlin.de/dailymed/

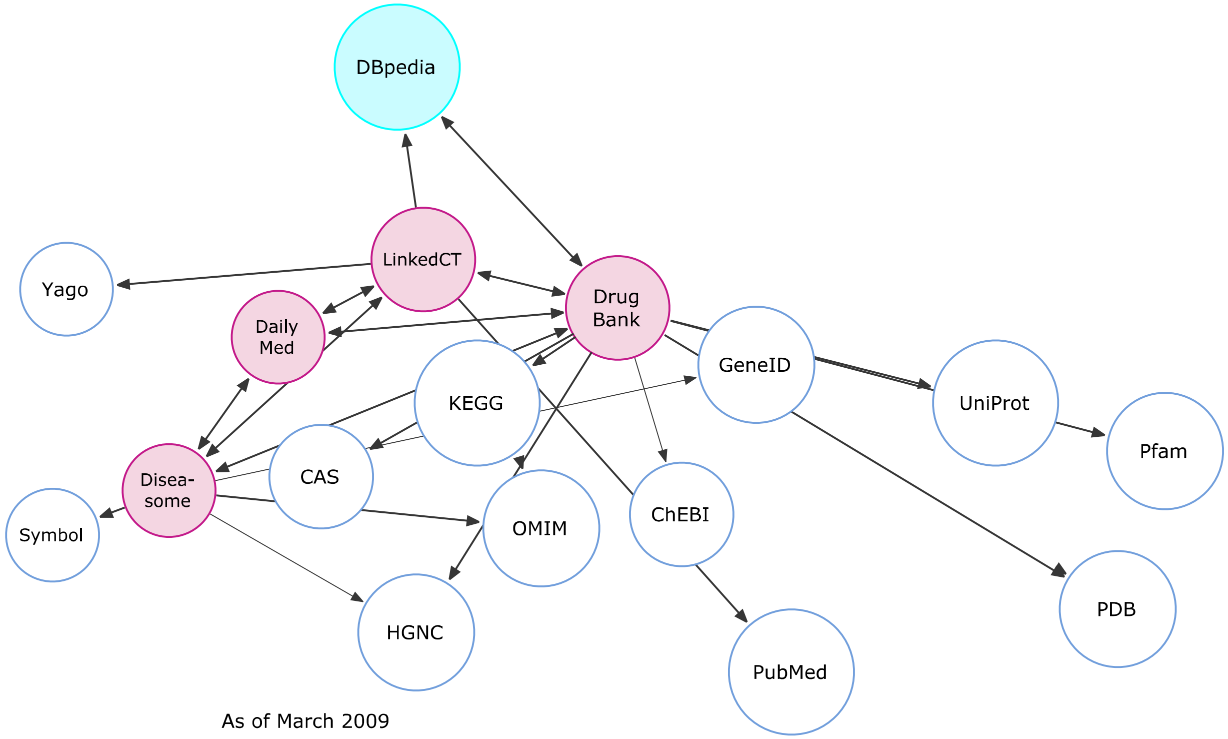
  - High quality information about marketed drugs
    - Published by the National Library of Medicine
    - In a flat file representation
  - 124,000 triples

- Diseasome

  http://www4.wiwiss.fu-berlin.de/diseasome/

  - Information about 4,300 disorders and disease genes linked by known disorder–gene associations
    - Published in Structured Product Labeling (an XML-based standard for exchanging medication information)
  - 88,000 triples

Interlinking Datasets



As of March 2009

- Two classes of links
  - Based on common identifiers
    - Links present in the source data sets
  - Based on link discovery and record linkage techniques
    - String matching
    - Semantic matching

Interlinking Datasets

- Link discovery techniques
  - String matching
    - Linking LinkedCT and Diseasome
      - E.g., "Alzheimer's disease" in LinkedCT was matched with "Alzheimer_disease" in Diseasome
  - Semantic matching
    - Many drugs and diseases have multiple names
      - E.g., "Varenicline" has the synonym "Varenicline Tartrate" and the brand names "Champix" and "Chantix"

Interlinking Statistics

Data set	Number of links
LinkedCT	290,000 links; 50,000 of them inside the LODD cloud
DrugBank	23,000 links; 8,500 of them inside the LODD cloud
DailyMed	29,600 links; all of them inside the LODD cloud
Diseasome	23,000 links; 8,400 of them inside the LODD cloud
Total	365,600 links; 8.4 million triples

Business Use Cases

- http://esw.w3.org/topic/HCLSIG/LODD/Business
- Example competitive intelligence use case
  - A neuroscience focused business manager interested in seeing an update on new clinical trials by competitors on Alzheimer's Disease (AD).
    - A phase III trial by Pfizer for a drug called Varenicline http://data.linkedct.org/resource/trials/NCT00744978
    - More information about the drug on DBpedia, DailyMed and DrugBank
      - http://dbpedia.org/resource/Varenicline
      - http://www4.wiwiss.fu-berlin.de/drugbank/resource/drugs/DB01273
    - DailyMed indicates the drug is already on the market for Nicotine addiction
      - Possible side effects are listed for the typical dose
      - According to LinkedCT, the dose in the trial is no more than the typical dose

Business Use Cases

- Why a nicotine addiction drug might work for AD?
  - DrugBank allows the manager to find drug targets “Neuronal acetylcholine receptor subunit alpha-4” and “Neuronal acetylcholine receptor subunit alpha-7” and associated gene names
  - Diseasome, however, indicates that the corresponding genes are only important in nicotine addiction, rather than AD.
  - This suggests that there is a more complex relationship between the diseases, than just sharing a drug target.
  - Extending the browsing to the SWAN Knowledgebase* shows that there are hypotheses relating AD to nicotinic receptors through amyloid beta.

  * http://hypothesis.alzforum.org/swan/

Conclusion and Future Work

- □ Extending the LOD cloud with HCLS datasets
  - Focus on clinical and pharmaceutical data sources
- □ Identify missing datasets and linkage points
  - By developing business use cases by pharmaceutical researchers
- □ Interlinking of the datasets
  - Using novel link discovery tools and frameworks including Silk and LinQuer
- □ Evaluating linked data exploration interfaces

The End

□ Thank you!