
Linking Up:

**An overview of the W3C Semantic Web Health
Care and Life Sciences
Interest Group**

**M. Scott Marshall
University of Amsterdam**

Birth of the HCLSIG

- **W3C Workshop on Semantic Web for Life Sciences, October 2004, Cambridge, MA, USA**
- **115 participants**
- **<http://www.w3.org/2004/07/swls-ws.html>**
- **HCLSIG Charter in early 2005**

Recharter in June 2008

- Co-chairs are Chimezie Ogbuji (Cleveland Clinic Foundation), M. Scott Marshall (University of Amsterdam), Susie Stephens (Eli Lilly)
- W3C team contact is Eric Prud'hommeaux (W3C)
- 85 formal participants across pharma, health care, academia, and technology companies
- Mailing list of >500 people

What is the Mission of HCLS IG?

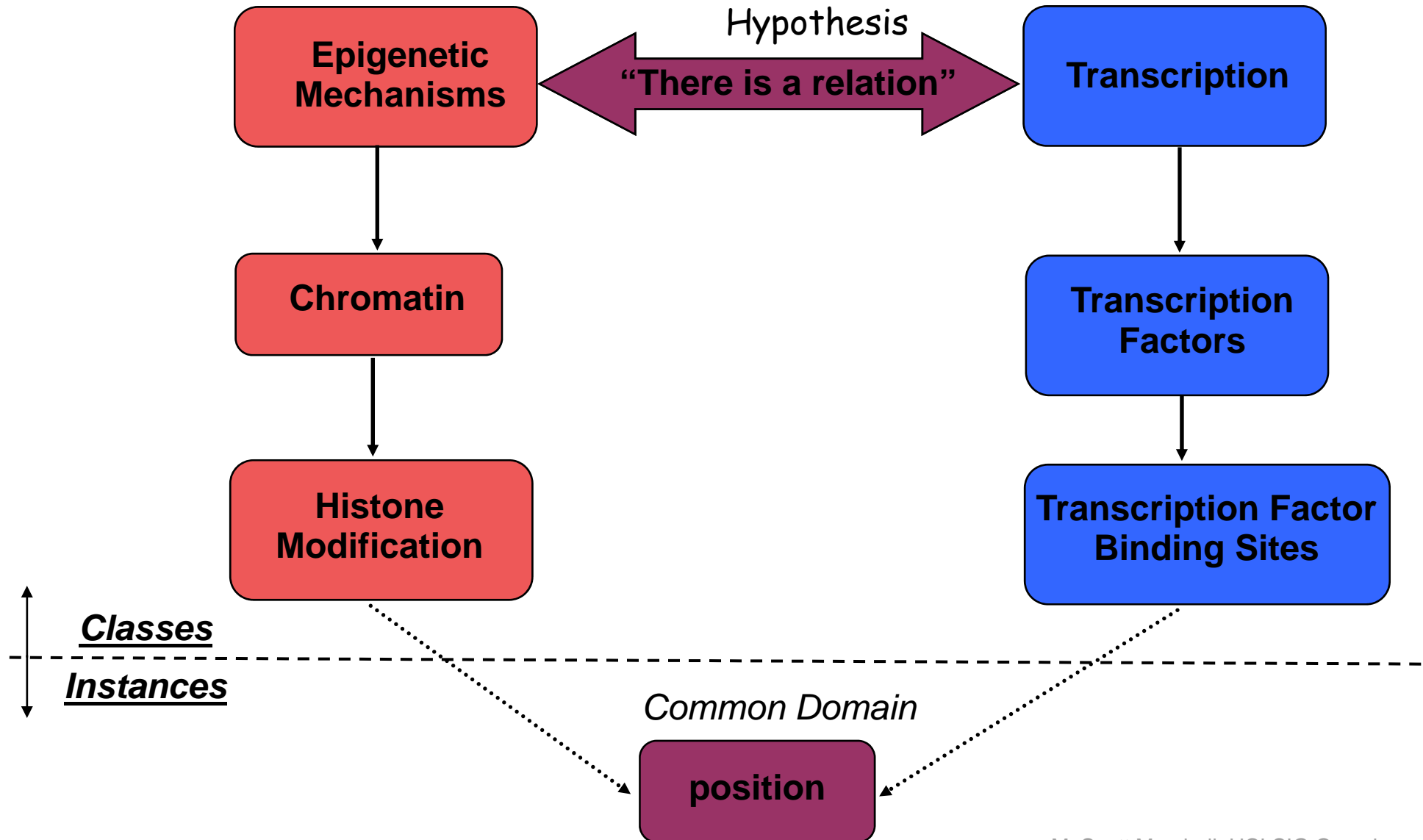
- The mission of the Semantic Web Health Care and Life Sciences Interest Group, part of the Semantic Web Activity, **is to develop, advocate, and support the use of Semantic Web technologies for biological science, translational medicine and health care.** These domains stand to gain tremendous benefit by adoption of Semantic Web technologies, as they depend on the interoperability of information from many domains and processes for efficient decision support.

Vision: Concept-based interfaces

- The scientist should be able to work in terms of ***commonly used*** concepts.
- The scientist should be able to work in terms of ***personal concepts*** and ***hypotheses***.
 - Not be forced to map concepts to the terms that have been chosen for a given application by the application builder.

Interface Sketch:

Finding a basis for relation



What does the group do?

- **Document use cases** to aid individuals in understanding the business and technical benefits of using Semantic Web technologies
- **Document guidelines** to accelerate the adoption of the technology
- **Implement** a selection of **the use cases** as proof-of-concept demonstrations
- Explore the possibility of **developing** high-level **vocabularies**
- **Disseminate information** about the group's work at government, industry, and academic events

HCLS IG Documents

W3C Interest Group Note

W3C

A Prototype Knowledge Base for the Life Sciences

W3C Interest Group Note 4 June 2008

This version:
<http://www.w3.org/TR/2008/NOTE-hcls-kb-20080604/>

Latest version:
<http://www.w3.org/TR/hcls-kb/>

Previous version:
<http://www.w3.org/TR/2008/WD-hcls-kb-20080404/>

Editors:
M. Scott Marshall, University of Amsterdam <marshall@science.uva.nl>
Eric Prud'hommeaux, W3C <eric@w3.org>

Contributors:
Alan Ruttenberg, Science Commons <alanruttenberg@gmail.com>
Jonathan Rees, Science Commons <jar@creativecommons.org>
Susie Stephens, Lilly <Stephens_Susie_M@lilly.com>
Matthias Samwald, Yale Center for Medical Informatics, DERI Galway, Semantic Web Company <samwald@gmx.at>
Kei-Hoi Cheung, Yale Center for Medical Informatics <kei.cheung@yale.edu>

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Abstract

The prototype we describe is a biomedical knowledge base, constructed for a demonstration at [Banff WWW2007](#), that integrates 15 distinct data sources using currently available Semantic Web technologies such as the W3C standard Web Ontology Language [OWL] and Resource Description Framework [RDF]. This report outlines which resources were integrated, how the knowledge base was constructed using free and open source triple store technology, how it can be queried using the W3C Recommended RDF query language SPARQL [SPARQL], and what resources and inferences are involved in answering complex queries. While the utility of the knowledge base is illustrated by identifying a set of genes involved in Alzheimer's Disease, the approach described here can be applied to any use case that integrates data from multiple domains.

Experiences with the conversion of SenseLab databases to RDF/OWL - Microsoft Internet Explorer provided by EB Lilly and Cospan

W3C Interest Group Note

W3C

Experiences with the conversion of SenseLab databases to RDF/OWL

W3C Interest Group Note 4 June 2008

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<http://www.w3.org/TR/2008/NOTE-hcls-senselab-20080604/>

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Editors:
Matthias Samwald, Yale Center for Medical Informatics / DERI Galway / Semantic Web Company <samwald@gmx.at>
Kei-Hoi Cheung, Yale Center for Medical Informatics <kei.cheung@yale.edu>


Contributors:
Alan Ruttenberg, Science Commons <alanruttenberg@gmail.com>
HuaJun Chen, Yale Center for Medical Informatics / Zhejiang University <hua.jun.chen@yale.edu>

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Abstract

One of the challenges facing Semantic Web for Health Care and Life Sciences is that of converting relational databases into Semantic Web format. The issues and the steps involved in such a conversion have not been well documented. To this end, we have created this document to describe the process of converting SenseLab databases into OWL. SenseLab is a collection of relational (Oracle) databases for neuroscientific research. The conversion of these databases into RDF/OWL format is an important step towards realizing the benefits of Semantic Web in integrative neuroscience research. This document describes how we represented some of the SenseLab databases in Resource Description Framework (RDF) and Web Ontology Language (OWL), and discusses the advantages and disadvantages of these representations. Our OWL representation is based on the reuse and extension of existing standard OWL ontologies developed in the biomedical ontology communities. The purpose of this document is to share our implementation experience with the community.

HCLS Web Site



Semantic Web Health Care and Life Sciences (HCLS) Interest Group

Introduction

The **mission** of the Semantic Web Health Care and Life Sciences Interest Group, part of the [Semantic Web Activity](#), is to develop, advocate for, and support the use of Semantic Web technologies for biological science, translational medicine and health care. These domains stand to gain tremendous benefit by adoption of Semantic Web technologies, as they depend on the interoperability of information from many domains and processes for efficient decision support.

The group will:

- Document use cases to aid individuals in understanding the business and technical benefits of using Semantic Web technologies.
- Document guidelines to accelerate the adoption of the technology.
- Implement a selection of the use cases as proof-of-concept demonstrations.
- Explore the possibility of developing high level vocabularies.
- Disseminate information about the group's work at government, industry, and academic events.

Participation

Communications of the HCLS IG are public. This includes public meeting records and access to the archives of the public-semweb-lifesci@w3.org mailing list.

The HCLS IG welcomes active participation from representatives of W3C Member organizations. If you are part of a W3C Member organization and you already have a W3C user account, you can join the HCLS IG by filling in the [participation form](#). Otherwise, please follow the instructions on [how to become a W3C Member](#). Active participation means participating at the weekly phone meetings, joining the discussions on the mailing list and, possibly, and participating at the face to face meetings.

Links

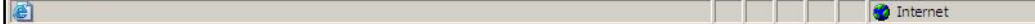
- Interest Group links:
 - [Group Charter](#)
 - [Public Wiki page](#)
- Participants:
 - [organizations](#)
 - [persons](#) (member only link)
- [Mailing list archives](#)
- Previous documents:
 - [A Prototype Knowledge Base for the Life Sciences](#)
 - [Experiences with the conversion of SenseLab databases to RDF/OWL](#)
- Other links:
 - [Semantic Web Activity Home](#)
 - [Previous Charter](#)

News Search

☒ All Words
☐ Some Word
☐ Entire phrase

News Categories

- [All](#)
- [group logistics](#) (2)



HCLS Wiki

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FrontPage RecentChanges FindPage HelpContents **HCLSIG**

Edit (Text) Edit (GUI) Info Subscribe Add Link Attachments More Actions:

Semantic Web for Health Care and Life Sciences Interest Group

The [mission of the Semantic Web for Health Care and Life Sciences Interest Group \(HCLSIG\)](#) is to develop, advocate for, and support the use of Semantic Web technologies for biological science, translational medicine and health care. These domains stand to gain tremendous benefit by adoption of Semantic Web technologies, as they depend on the interoperability of information from many domains and processes for efficient decision support. More information on the group is available on the [W3C Web site for the HCLSIG](#).

HCLSIG Group Meetings

Telcon

- [Next Meeting October 2](#)
- [Past Meetings](#)

F2F

- [/F2F/2008-10 F2F](#)

Task Forces

Group	Time (UTC)	Code	IRC
HCLSIG	Thu 1500	HCLS	#hcls
Current Task Forces			
BioRDF	Mon 1500	BioRDF	#BioRDF
Clinical Decision Support			
Clinical Observations Interoperability	Tue 1500	BioONT	#hcls
Linking Open Drug Data	Wed 1500	HCLS	#hcls
Scientific Discourse	Fri 1500	HCLS	#hcls
Terminology			

Motivation for New Members

- **Benefits to getting involved include:**
 - early access to use cases and best practice
 - influence standard recommendations
 - cost effective exploration of new technology through collaboration
 - network with others working with Semantic Web
- **Get involved by contacting the chairs:**
 - team-hcls-chairs@w3.org

Meetings

- Formal F2F, January 2006, Cambridge
- Formal F2F, October 2006, Amsterdam
- Workshop, ISWC November 2006, Banff
- Informal F2F (Demo) 3 x March/April, 2007, Cambridge
- Workshop, WWW 2007, May 2007, Banff
- Informal F2F (URI), July 2007, Cambridge
- Formal F2F, November 2007, Cambridge
- Formal F2F, October 2008, Mandelieu
- (You are HERE)

Publications

Submitted:

- **Life Sciences on the Semantic Web: The Neurocommons and Beyond**

Alan Ruttenberg, Jonathan Rees, Matthias Samwald, M. Scott Marshall

In Print:

- **Advancing translational research with the Semantic Web**

Alan Ruttenberg, Tim Clark, William Bug, Matthias Samwald, Olivier Bodenreider, Helen Chen, Donald Doherty, Kerstin Forsberg, Yong Gao, Vipul Kashyap, June Kinoshita, Joanne Luciano, M Scott Marshall, Chimezie Ogbuji, Jonathan Rees, Susie Stephens, Gwendolyn T Wong, Elizabeth Wu, Davide Zaccagnini, Tonya Hongsermeier, Eric Neumann, Ivan Herman and Kei-Hoi Cheung, BMC Bioinformatics 2007, 8(Suppl 3):S2

- **An Ontology-based approach for Data Integration - An Application in Biomedical Research**

Vipul Kashyap, Kei-Hoi Cheung, Don Doherty, Matthias Samwald, M. Scott Marshall, Joanne Luciano, Susie Stephens, Ivan Herman and Ray Hookway, Book Chapter in Cardoso, J., Hepp, M., Lytras, M. (Eds.) "Real-world Applications of Semantic Web Technology and Ontologies", Springer 2007.

Presentations -> 2007

- **WWW2007 Demo**
- **ISMB 2007 Demo**
- **ISMB BioOntology SIG Poster 2007**
- **Society for Neuroscience Poster Nov 2007**
- **Selection of presentation venues of members showing HCLS work**
 - **Bridging Pharma and IT**
 - **Drug Discovery Technology of Innovative Therapeutics**
 - **1st European Semantic Web Conference**
 - **Bio-IT World**
 - **Norwegian Semantic Web Day**
 - **InfoTech Pharma**
 - **Modern Drug Discovery and Development Summit**
 - **Massachusetts Biotechnology Panel**
 - **eScience Institute; RDF, Ontologies and Meta-Data Workshop**
 - **Virginia Biotechnology Summit**
 - **Systems Biology**
 - **Semantic Web Gathering**
 - **Allen Institute for Brain Sciences**
 - **Informatics and Interactomes in Huntington's Disease**
 - **Ontology for Biomedical Informatics Workshop**
 - **Clinical Trial Ontology Workshop**
 - **Jackson Laboratories**
 - **Pubmed Plus**
 - **NIH Blueprint NIF Workshop**

Presentations in 2008

- Asian Semantic Web Conference, HCLS Workshop
- ISWC 2008 Semantic Web for Health Care and Life Sciences Tutorial
- SWAT4LS 2008 Workshop
- Reasoning Web Summer School 2008
- WWW2008 Workshop
- ISMB 2008 Demo
- Selection of presentation venues of members showing HCLS work:
 - ☐ Drug Discovery Technology of Innovative Therapeutics
 - ☐ European Semantic Web Conference
 - ☐ Bio-IT World
 - ☐ InfoTech Pharma 2008
 - ☐ ...

Linked Data Principles



- 1. Use URIs as names for things.**
- 2. Use HTTP URIs so that people can look up those names.**
- 3. When someone looks up a URI, provide useful RDF information.**
- 4. Include RDF statements that link to other URIs so that they can discover related things.**

- Tim Berners-Lee 2007
- <http://www.w3.org/DesignIssues/LinkedData.html>

Task Forces

- **BioRDF** – integrated neuroscience knowledge base
 - Task lead - **Kei Cheung**
- **Clinical Decision Support** – expression and use of guidelines
 - Task lead – TBD
- **Clinical Observations Interoperability** – patient recruitment in trials
 - Task lead - **Vipul Kashyap**
- **Linking Open Drug Data** – aggregation of Web-based drug data
 - Task lead - Chris Bizer
- **Scientific Discourse** – building communities through networking
 - Task leads - **Tim Clark, John Breslin**
- **Terminology** – Semantic Web representation of existing resources
 - Task lead - **John Madden**

BioRDF Task

- **BioRDF participants**
 - The task is lead by Kei Cheung (Yale)
 - Has approximately 20 participants
- **BioRDF activities include:**
 - Explore the effectiveness of current tools for making data available as RDF/OWL
 - Build a life sciences demo that spans from bench to bedside using RDF/OWL to help scientist better understand the value of the Semantic Web
 - Document our finding to help accelerate the adoption of the Semantic Web by others
- **BioRDF Publications**
 - A Prototype Knowledge Base for the Life Sciences - <http://www.w3.org/TR/hcls-kb/>
 - Experience with the Conversion of SenseLab Databases to RDF/OWL – <http://www.w3.org/TR/hcls-senselab/>
- **More Information on the group is available at**
 - http://esw.w3.org/topic/HCLSIG_BioRDF_Subgroup

BioRDF - Answering Questions

- **Goals:** Get answers to questions posed to a body of collective knowledge in an effective way
- **Knowledge used:** Publicly available databases, and text mining
- **Strategy:** Integrate knowledge using careful modeling, exploiting Semantic Web standards and technologies

COI Goals

- **Demonstrate the value of Semantic Web specifications to bridge the divide between clinical practice and clinical research**
- **Develop collaboratively a proof of concept**
- **Get a variety of stakeholders to participate as a prelude to acceptance and adoption**

COI Use Cases

- **Wide variety of use cases were investigated and discussed**
 - **Patient Recruitment**
 - **Adverse Event Detection**
 - **Tracking Patient Through a Clinical Trial**
- **Decision: Focus on Patient Recruitment**

Linking Open Drug Data (LODD)

Primary Objectives

- 1. Survey publicly available data sets about drugs**
- 2. Explore how the data sets could be linked together**
- 3. Explore interesting questions that could be answered if the data sets are linked**

LODD Participants

- **Kristin Tolle (Microsoft)**
- **Eric Prud'hommeaux (W3C)**
- **Don Doherty (Brainstage)**
- **Susie Stephens (Lilly)**
- **Bosse Anderssen (AZ)**
- **M. Scott Marshall (University of Amsterdam)**
- **Chris Bizer (Freie Universitat Berlin)**
- **Glen Newton (National Research Council Canada)**
- **Michel Dumontier (Carleton University)**
- **TN Bhat (NIST)**

Data Sets for the LODD Task

- ClinicalTrials.gov
- LillyTrials
- Orange Book
- RxNorm
- Drug Bank
- Diseasome
- Drugome
- OMIM
- DrugDB
- Drug Ontology
- PubChem
- chEBI
- National Drug Code
- ChemBlast
- KEGG Drug
- VA NDF-RT

Plus ca change..

..plus c'est la meme chose.

- **Models change:**
 - **Epigenetics: The code isn't only in the DNA**
 - **Polypharmacology: We should aim for ligands with multiple targets.**
- **Terminologies change:**
 - **In Personal Medical Records:**
 - **Per user: patient, clinician**

Why Synonym Services?

Example: CBP has now officially been renamed KAT3A
p300 is now KAT3B

*See new nomenclature rules for chromatin remodellers: Cell,
Vol 131, 633-636, 16 November 2007*

Some common themes

- **Mapping from Terminology to Model**
- **Mapping from Terminology to Terminology**
- **Mapping from Model to Model**
- **...**

Raises some questions:

- **What to use for the mapping representation?**
- **How do we create the mapping/alignment?**

AIDA Search - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://aida.science.uva.nl:9999/search/test/search.htm

Wikipedia lookup FoaF Explorer Add To Connotea W3C Member Site W3C Semantic We... Microarrays Huntington's Semantic Metadata

AIDA Search

Search:

[Responses of the L5178Y tk+/tk- mouse lymphoma cell forward mutation assay: III. 72 coded chemicals.](#)
, 1,2-epoxyhexadecane, ethyl acrylate, ethyl benzene, ethylene thiourea, F D and C yellow Number 6... obtained with allyl isothiocyanate, p-benzoquinone dioxime, benzyl acetate, 2-biphenylamine HCl, bis
[cached](#)

[The mutagenic activity of 61 agents as determined by the micronucleus, Salmonella, and sperm abnormality assays.](#)
methane sulfonate (MMS); N-methyl-N-nitro-N'-nitrosoguanidine; Mitomycin C; Monosodium glutamate... is presented for 61 agents; Acetylsalicylic acid; Acriflavine; Actinomycin D; 2(2-furyl)-3
[cached](#)

[Polycyclic aromatic hydrocarbon profile analysis of high-protein foods, oils, and fats by gas chromatography.](#)
, fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzo(b)fluoranthene + benzo(j)fluoranthene + benzo(k)fluoranthene, benzo(e)pyrene, benzo(a)pyrene, perylene, dibenz(a,i)anthracene, dibenz(a,h)anthracene
[cached](#)

[Aryl hydrocarbon receptor-mediated activity of mutagenic polycyclic aromatic hydrocarbons determined using in vitro reporter gene assay.](#)
, dibenzo(a,h)anthracene, benzo(a)pyrene, dibenzo(a,i)anthracene, chrysene, and benzo(b)fluoranthene. High..., indeno(1,2,3-cd)pyrene, benzo(j)fluoranthene, dibenzo(a,e)fluoranthene and dibenzo(a,i)pyrene. These data
[cached](#)

[Ability of polycyclic aromatic hydrocarbons to induce 7-ethoxyresorufin-o-deethylase activity in a trout liver cell line.](#)
. The order of potency, from most to least potent, was benzo(k)fluoranthene, dibenzo(a,i)pyrene, dibenzo(a,h)anthracene, benzo(a)pyrene, indeno(1,2,3-cd)pyrene, benzo(b)fluoranthene, pentacene, benzo
[cached](#)

[Dose-response curves for liver DNA fragmentation induced in rats by sixteen N-nitroso compounds as measured by viscometric and alkaline elution analyses.](#)
-nitrosomethylethylamine (0.025 mg/kg), N-nitrosodiethylamine (0.067 mg/kg), N-nitrosodiethanolamine (1.03 mg/kg), N-nitrosodi-n-propylamine (0.31 mg/kg), N-nitrosodi-n-butylamine (0.083 mg/kg), N-nitroso-N
[cached](#)

[Photomutagenicity of 16 polycyclic aromatic hydrocarbons from the US EPA priority pollutant list.](#)
, benz(a)anthracene, benzo(ghi)perylene, benzo(a)pyrene, indeno(1,2,3-cd)pyrene, and pyrene. Under... are weakly photomutagenic. Benzo(b)fluoranthene, fluoranthene, naphthalene, phenanthrene, and dibenz(a,h

AIDA Thesaurus browser

Enter a term to search for...

- root
 - food and feed
 - feed
 - food
 - ingestion
 - hazards
 - hazards by effect
 - allergens
 - probable carcinogens
 - 1 1 1 2-tetrachloroethane
 - 1 1 1-trichloroethane
 - 1 1 2 2-tetrachloroethane
 - 1 1 2-trichloroethane
 - 1 1-dimethylhydrazine
 - 1 2 3-trichloropropane
 - 1 2-bis(chloromethoxy)prope
 - 1 2-diamino-4-nitrobenzene
 - 1 2-dibromo-3-chloropropane
 - 1 2-dichloroethane
 - 1 2-dichloropropane
 - 1 2-diethylhydrazine
 - 1 2-dimethylhydrazine
 - 1 2-epoxybutane
 - 1 3-butadiene

Page 1 of 88599

Results 1 - 10 of 885983 for +(content:"1 1 1 2-tetrachloroethane" content:"1 1...

Find: ☐ Match case

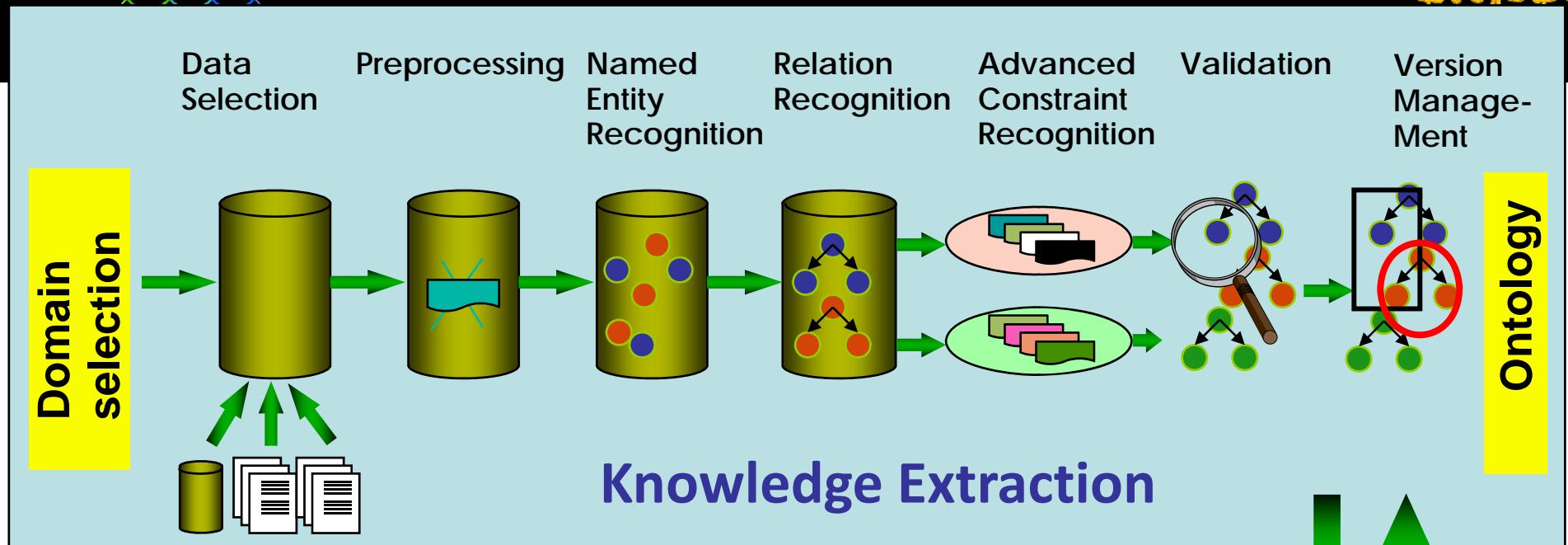
Done 4.110s 17 Errors

The Question Answering Process

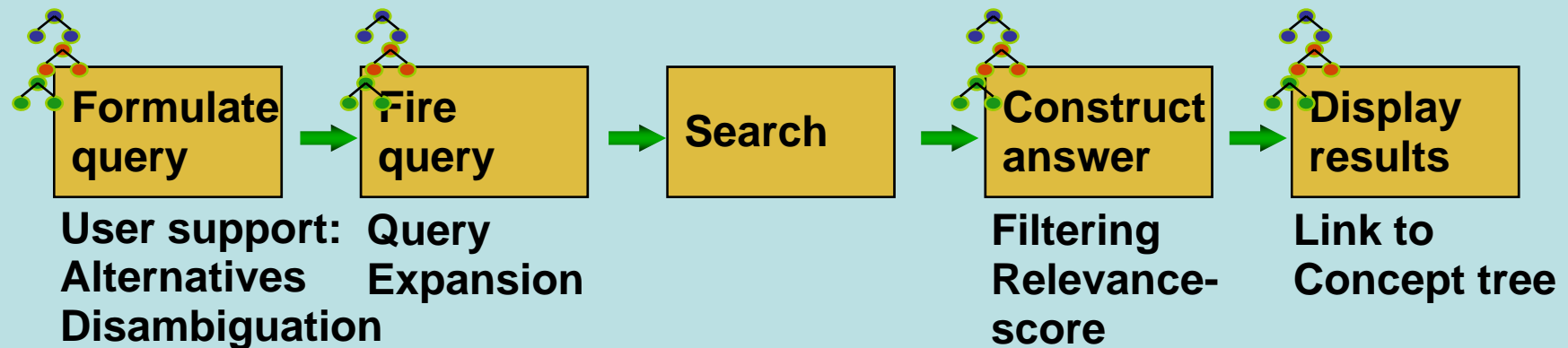
- **Start with terminology**
- **Translate into query language**
- **Query is compiled into a representation that can unify with the data representation**
- **➔ Add new knowledge to Knowledge Base**



Adaptive Information Disclosure



Information Retrieval



Scientific Question

“find me genes involved in signal transduction that are related to pyramidal neurons”

A SPARQL query for processes involved in pyramidal neurons

```
prefix go: <http://purl.org/obo/owl/GO#>
prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix mesh: <http://purl.org/commons/record/mesh/>
prefix sc: <http://purl.org/science/owl/sciencecommons/>
prefix ro: <http://www.obofoundry.org/ro/ro.owl#>

select ?genename ?processname
where
{
  graph <http://purl.org/commons/hcls/pubmesh>
  {
    ?paper ?p mesh:D017966 .
    ?article sc:identified_by_pmid ?paper.
    ?gene sc:describes_gene_or_gene_product_mentioned_by ?article.
  }
  graph <http://purl.org/commons/hcls/goa>
  {
    ?protein rdfs:subClassOf ?res.
    ?res owl:onProperty ro:has_function.
    ?res owl:someValuesFrom ?res2.
    ?res2 owl:onProperty ro:realized_as.
    ?res2 owl:someValuesFrom ?process.
  }
  graph <http://purl.org/commons/hcls/20070416/classrelations>
  {
    {{?process <http://purl.org/obo/owl/obo#part_of> go:GO_0007166}
    union
    {?process rdfs:subClassOf go:GO_0007166 }}
    ?protein rdfs:subClassOf ?parent.
    ?parent owl:equivalentClass ?res3.
    ?res3 owl:hasValue ?gene.
  }
  graph <http://purl.org/commons/hcls/gene>
  {
    ?gene rdfs:label ?genename
  }
  graph <http://purl.org/commons/hcls/20070416>
  {
    ?process rdfs:label ?processname
  }
}
```

Mesh: Pyramidal Neurons



Pubmed: Journal Articles

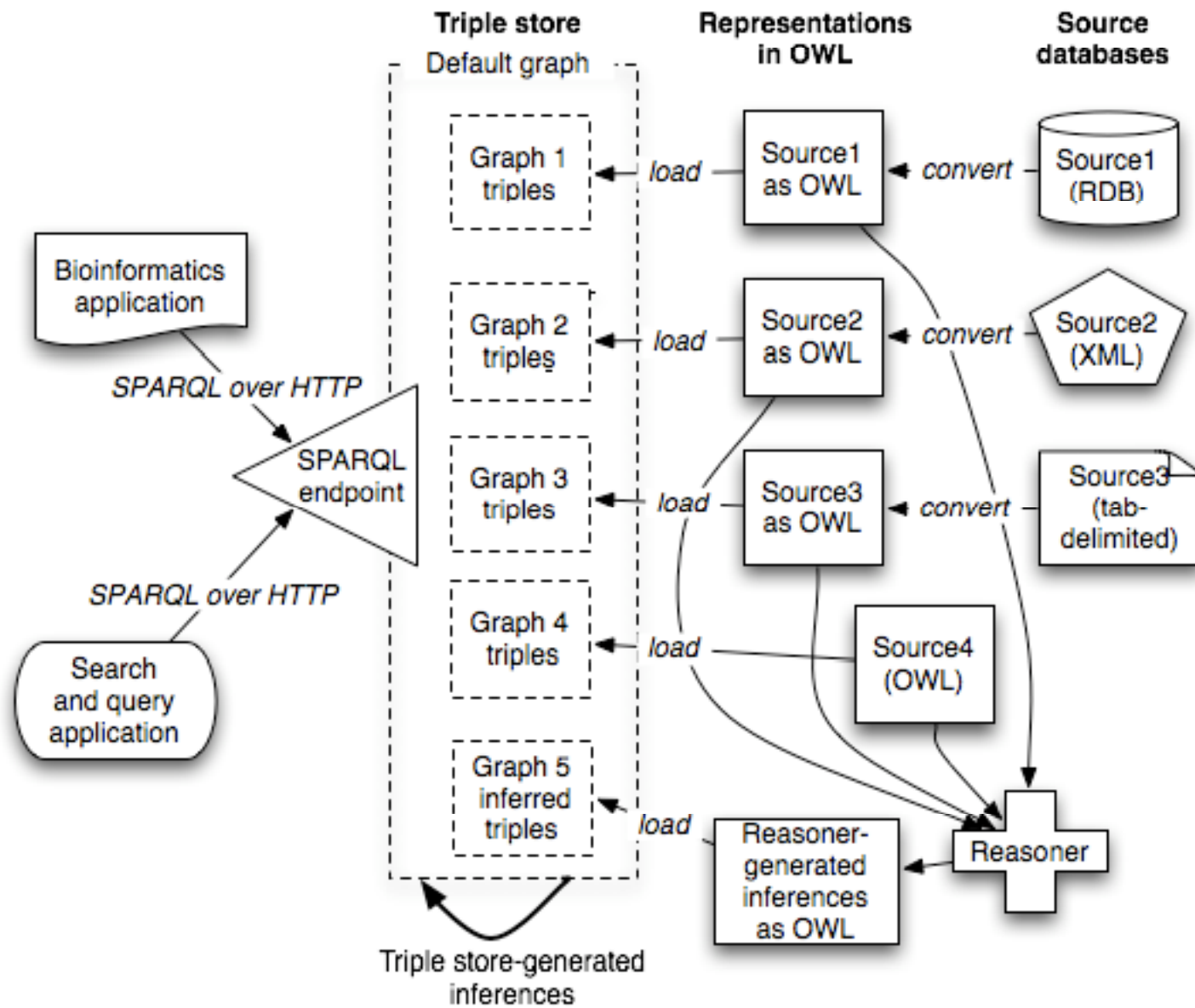


Entrez Gene: Genes



GO: Signal Transduction

Inference required



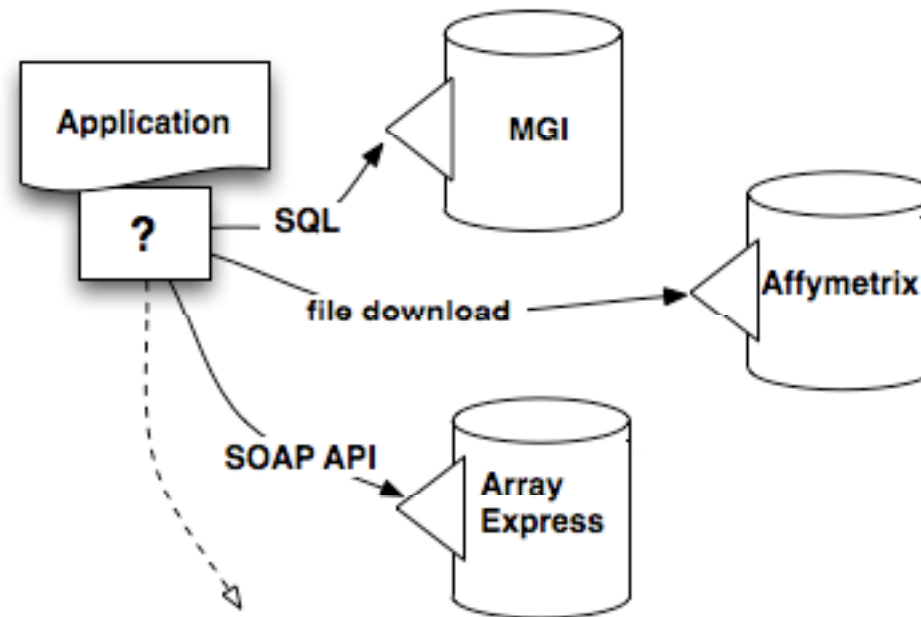
Next Phase

- **More Use Cases**
- **More Users (of Knowledge Base, our approaches)**
- **Store Knowledge in Rules**
- **Easier Interface**
 - Convenient term lookup from Knowledge Base
 - Automatic translation of terms in Interface
 - Saving and finding similar queries (collaborative filtering)
- **Distributed Knowledge (Queries)**
- **Reasoning across large Knowledge Bases**

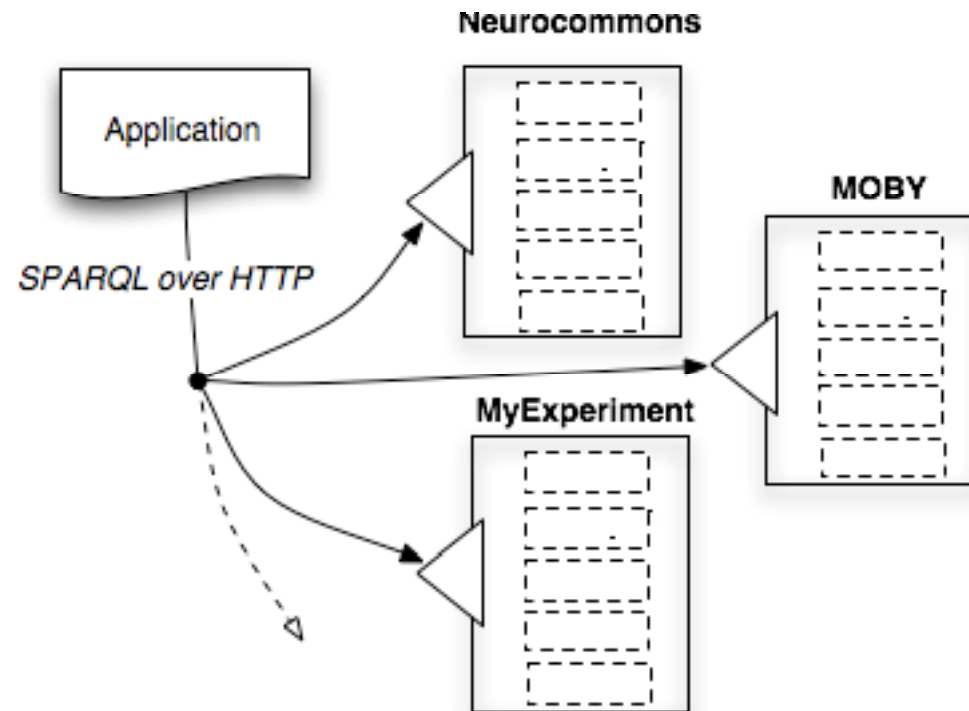
SPARQL-DL

```
1. SELECT ?gene_name ?process_name
2. WHERE
3. { PropertyValue(?pubmed_record, ?related, mesh:D017966)
4.   PropertyValue(?article, sc:identified_by_pmid , ?pubmed_record)
5.   PropertyValue(?gene_record, sc:describes_gene_or_gene_product_mentioned_by, ?article)
6.   SubClassOf(?protein, some(ro:has_function, some(ro:realized_as, ?process)))
7.   SubClassOf(?process, or(go:GO_0007166, some(ro:part_of, go:GO_0007166))
8.   SubClassOf(?protein, some(sc:is_protein_gene_product_of_dna_described_by, {?gene_record}))
9.   Annotation(?gene_record, rdfs:label, ?gene_name)
10.  Annotation(?process, rdfs:label, ?process_name)
11. }
```

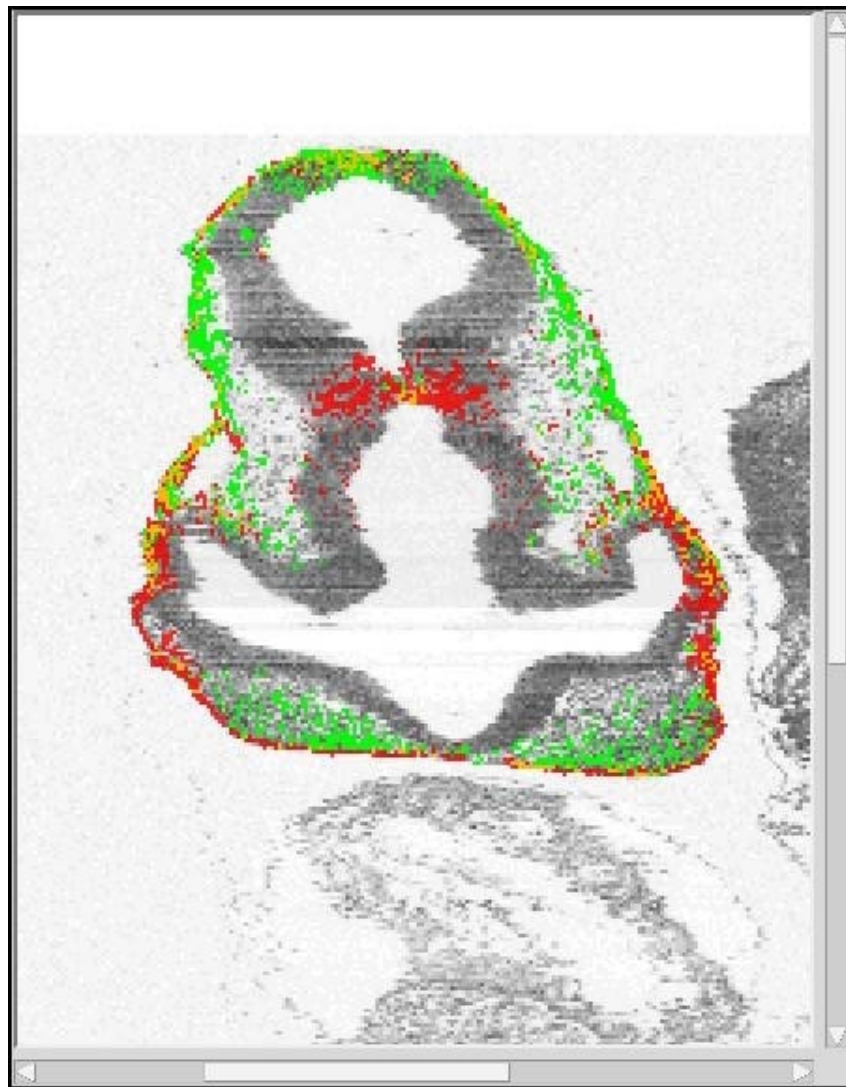
Distributed Query - Before



Distributed Query - After



**Someday, we should be able to find this as evidence for a fact in the
Knowledge Base**



The End

“Science is built up of facts, as a house is built of stones; but an accumulation of facts is no more a science than a heap of stones is a house.”

***– Henri Poincaré,
Science and Hypothesis, 1905***