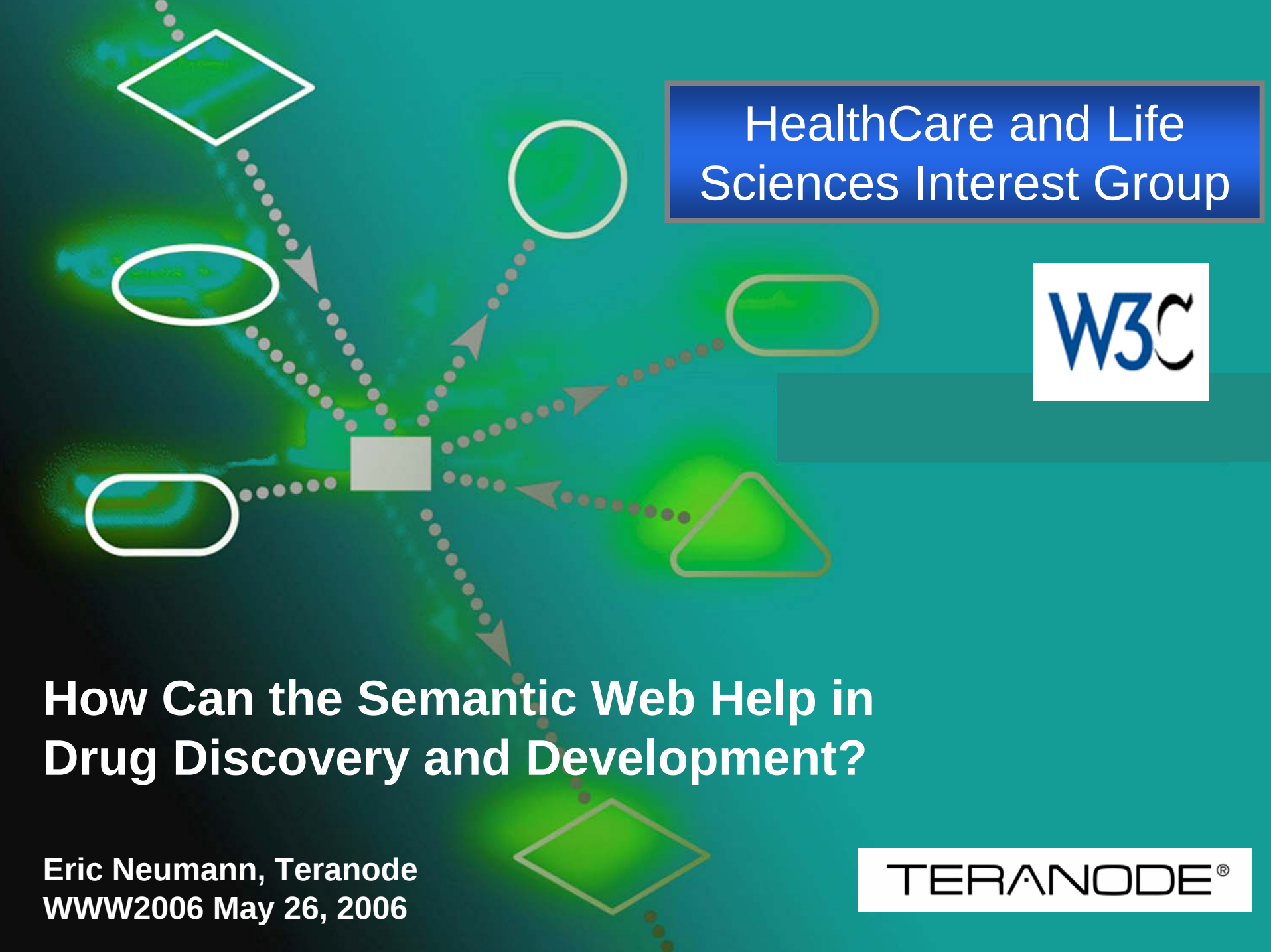




HealthCare and Life Sciences Interest Group

W3C

How Can the Semantic Web Help in Drug Discovery and Development?

Eric Neumann, Teranode
WWW2006 May 26, 2006

TERANODE®



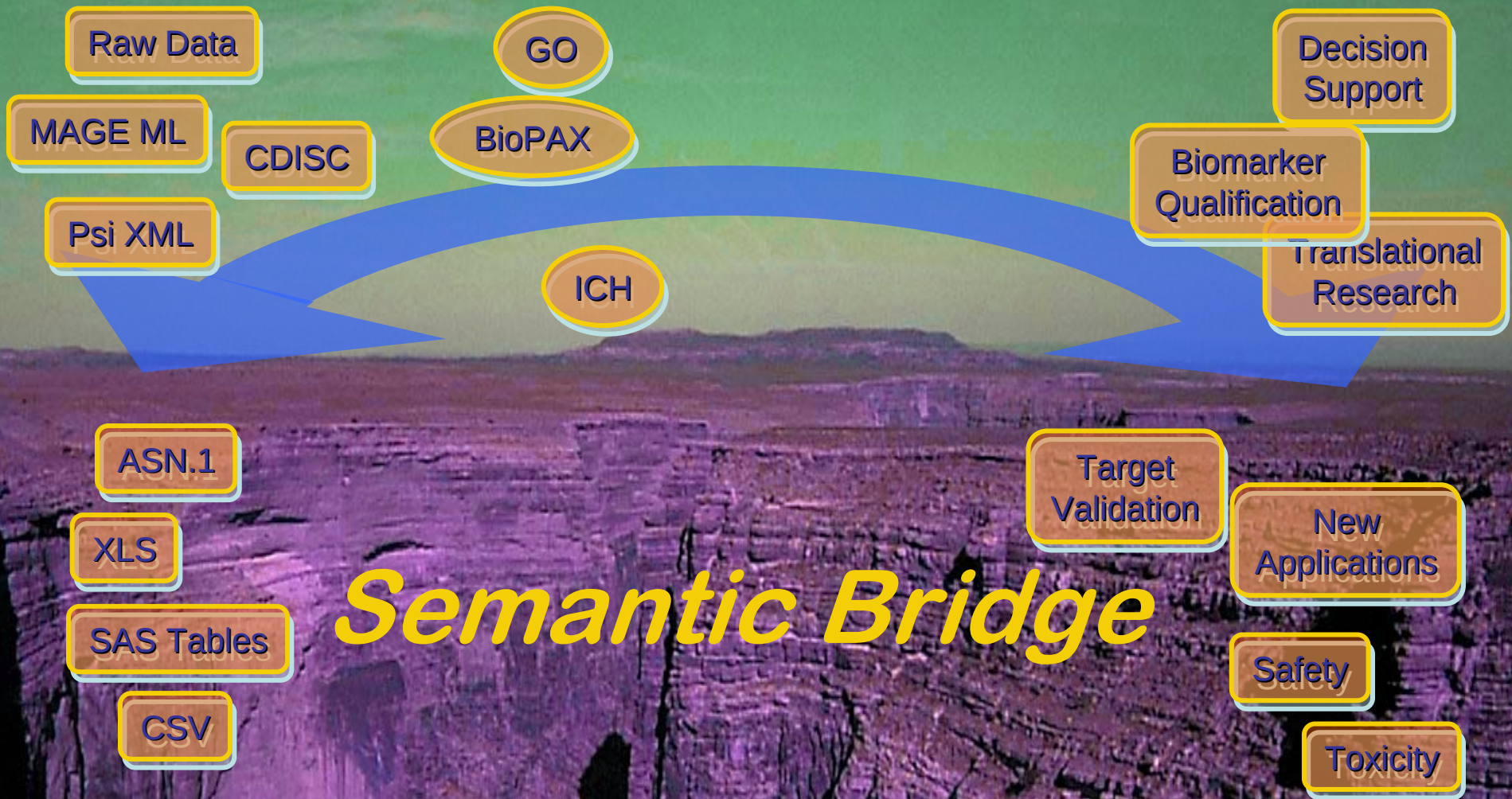
Drug Discovery and HealthCare

- *Health*
- *Practice*
- *Privacy*
- *Safety*
- *Prevention*
- *Knowledge*

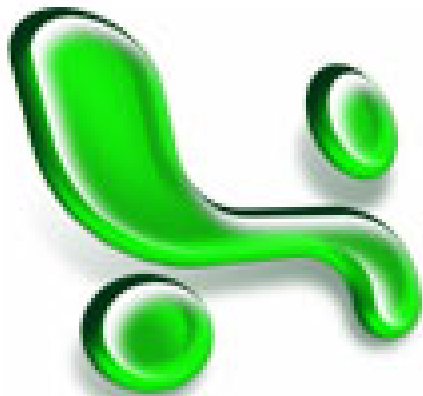
Where Information Advances are Most Needed



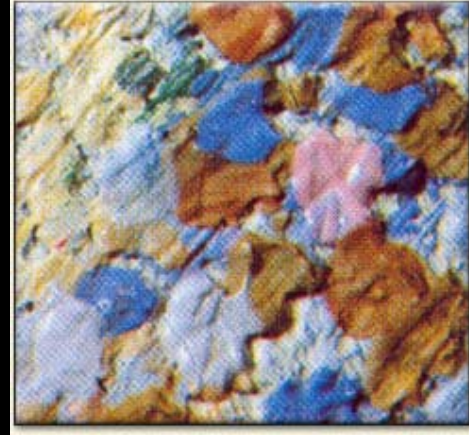
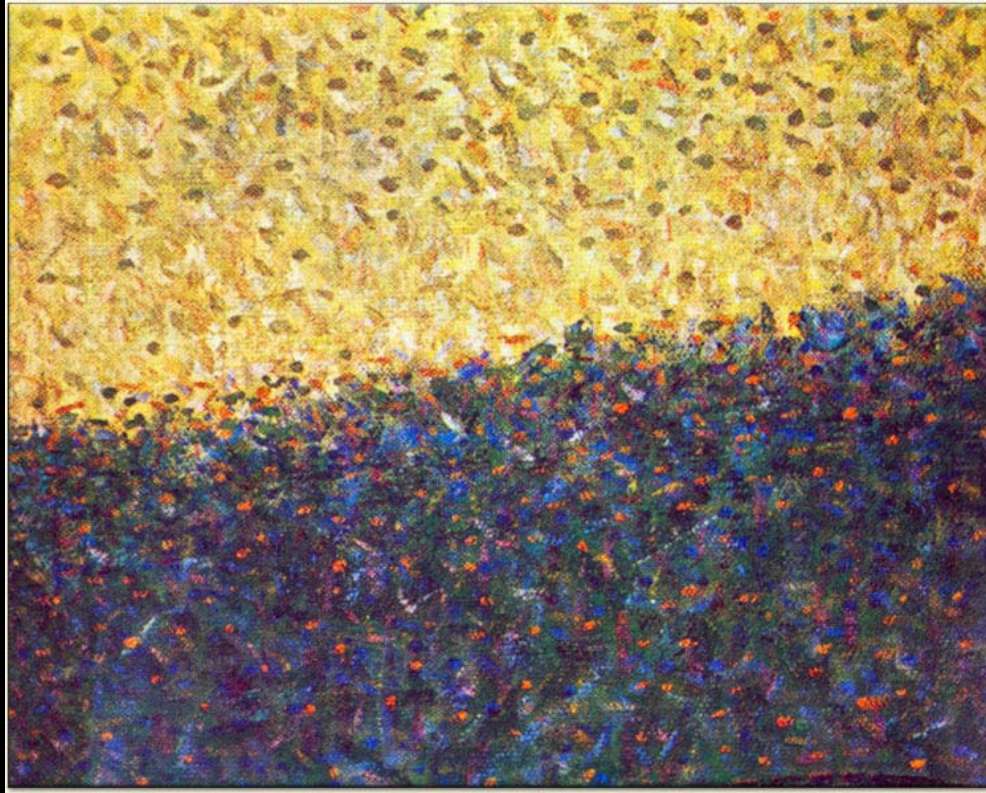
- Supporting Innovative Applications in R&D
 - Molecular Diagnostics (Biomarkers)
 - Molecular Mechanisms (Systems)
 - Data Provenance, Rich Annotation
- Clinical Information
 - Safety Information, Pharmacovigilance, Adverse Events
 - eHealth Records + EDC
 - Clinical Submission Documents
 - Handling Biomarker evidence
- Standards
 - Central Data Sources
 - Genomics, Diseases, Chemistry, Toxicology
 - MetaData
 - Ontologies
 - Vocabularies



Main Technologies for Exchanging Knowledge



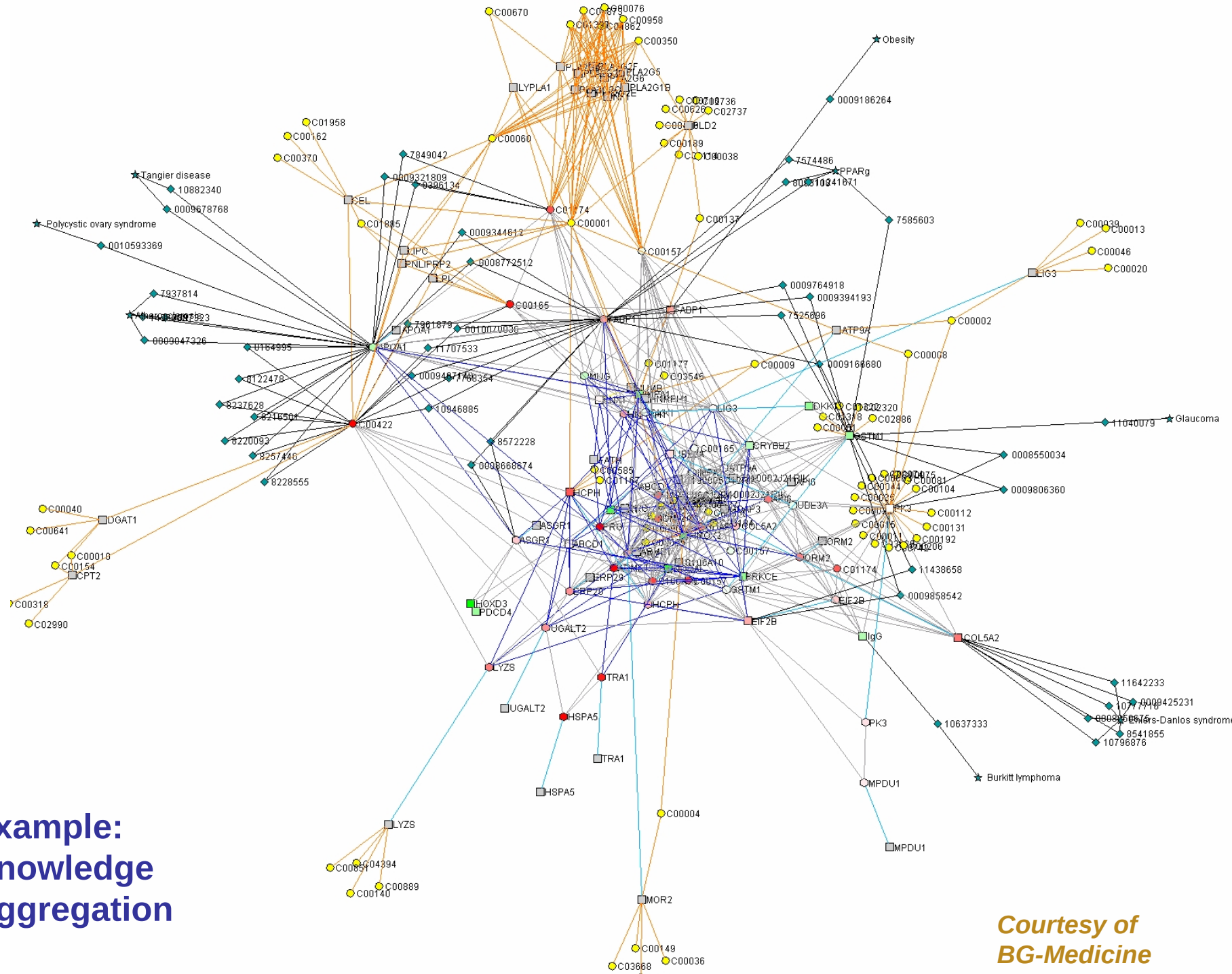
The Big R&D Picture -



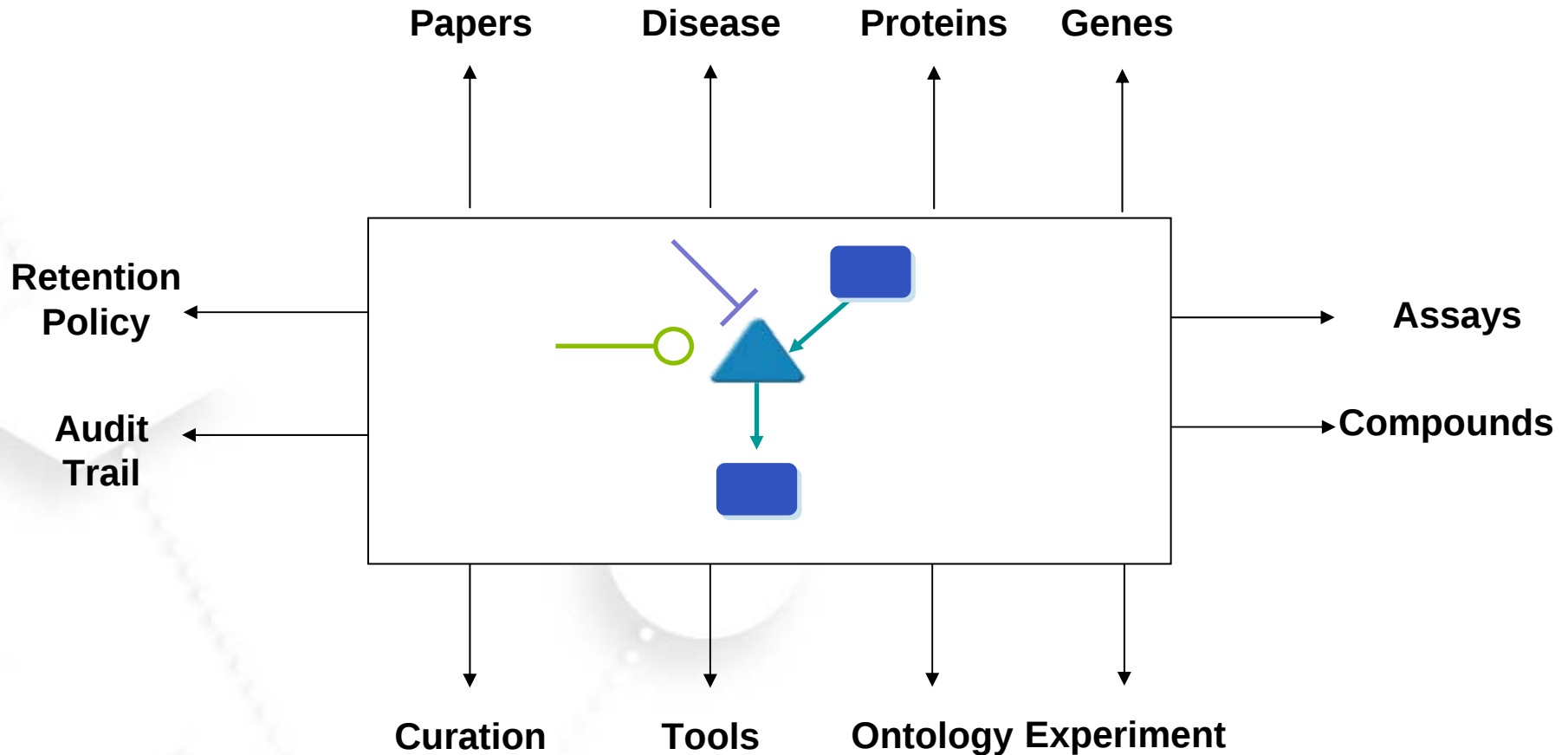
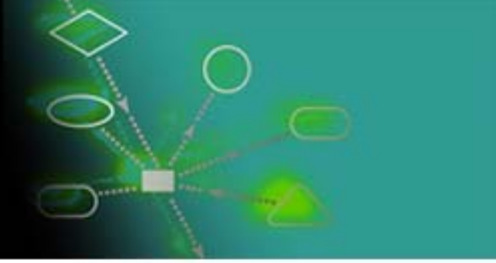
**Hard to understand from
just a few Points of View**



Complete view tells a very different Story



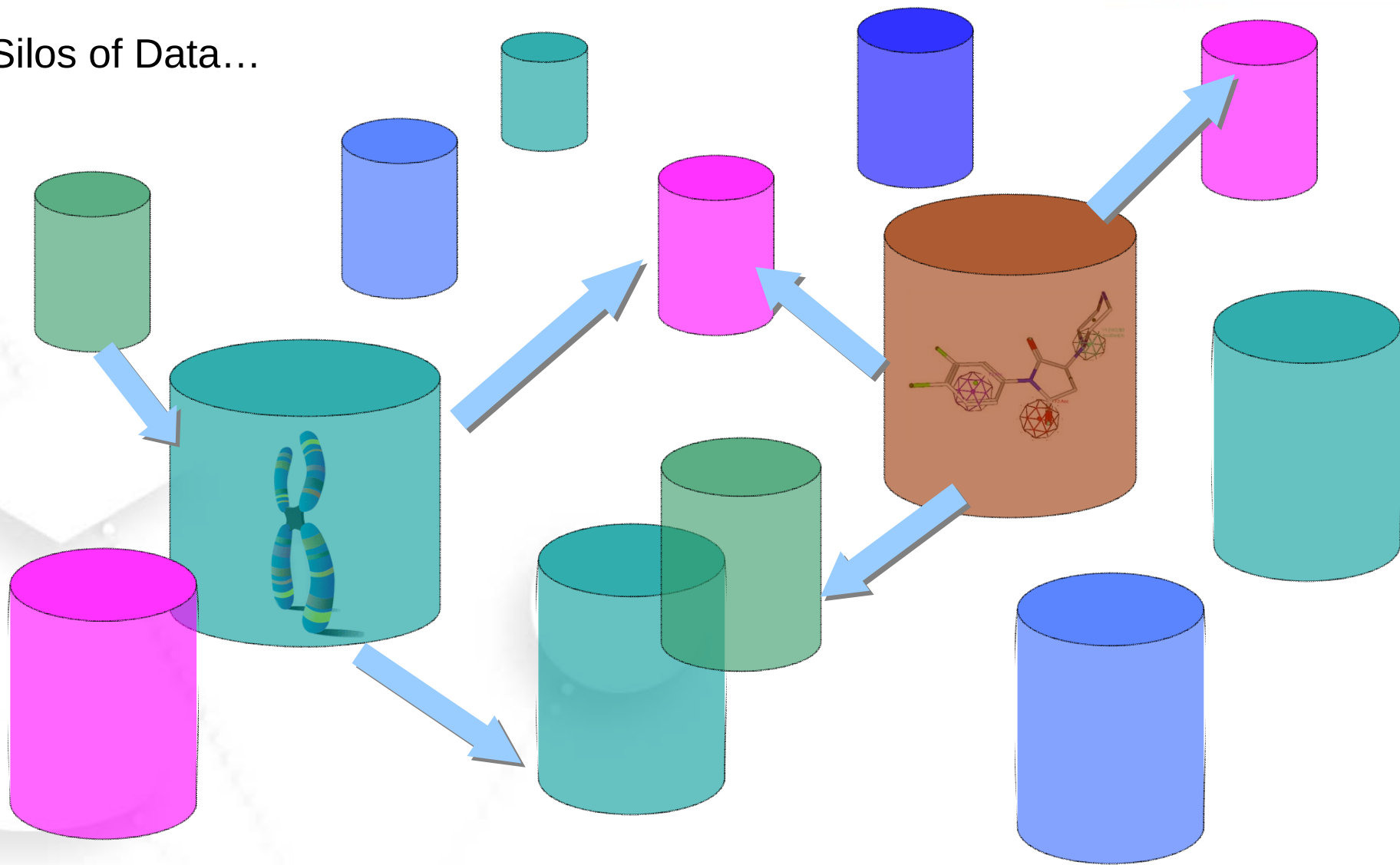
Data Integration: Biology Requirements



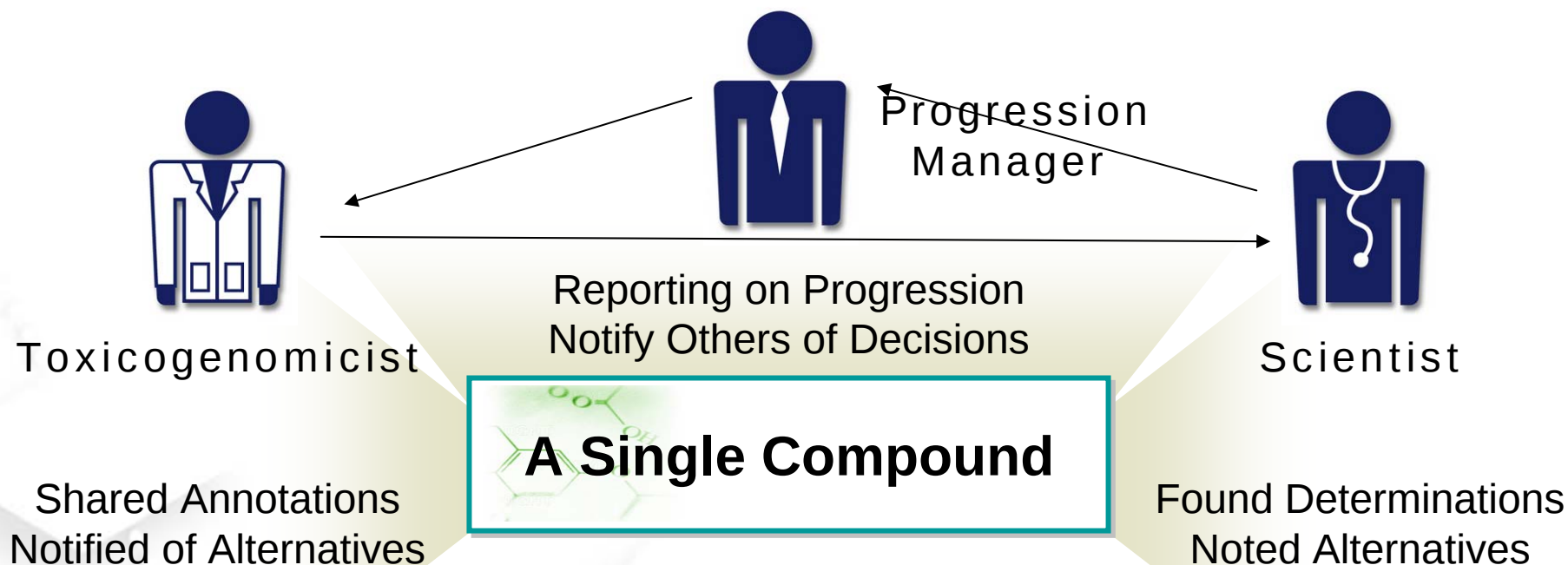
Distributed Nature of R&D



Silos of Data...

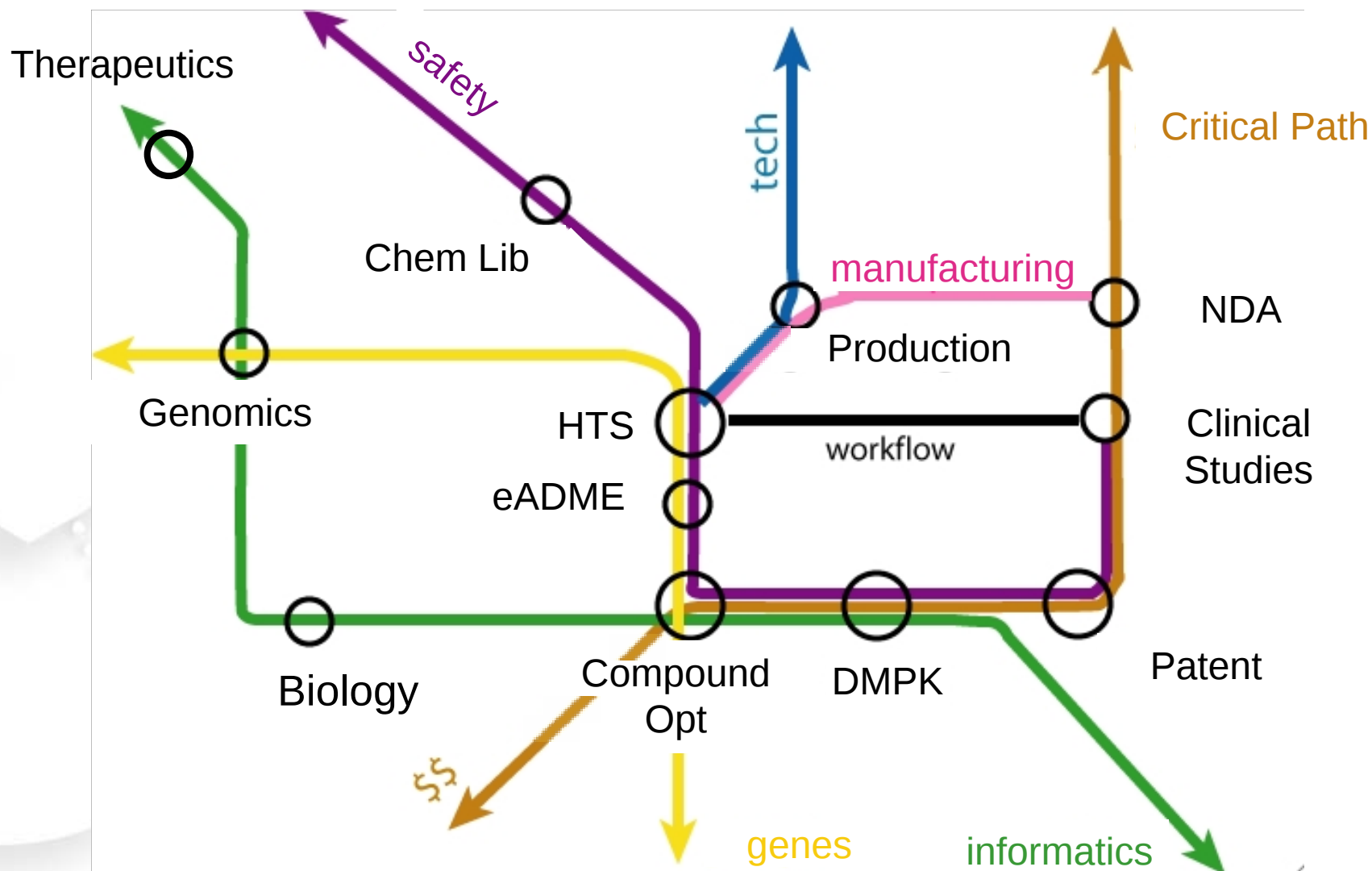


Semantic Web in R&D

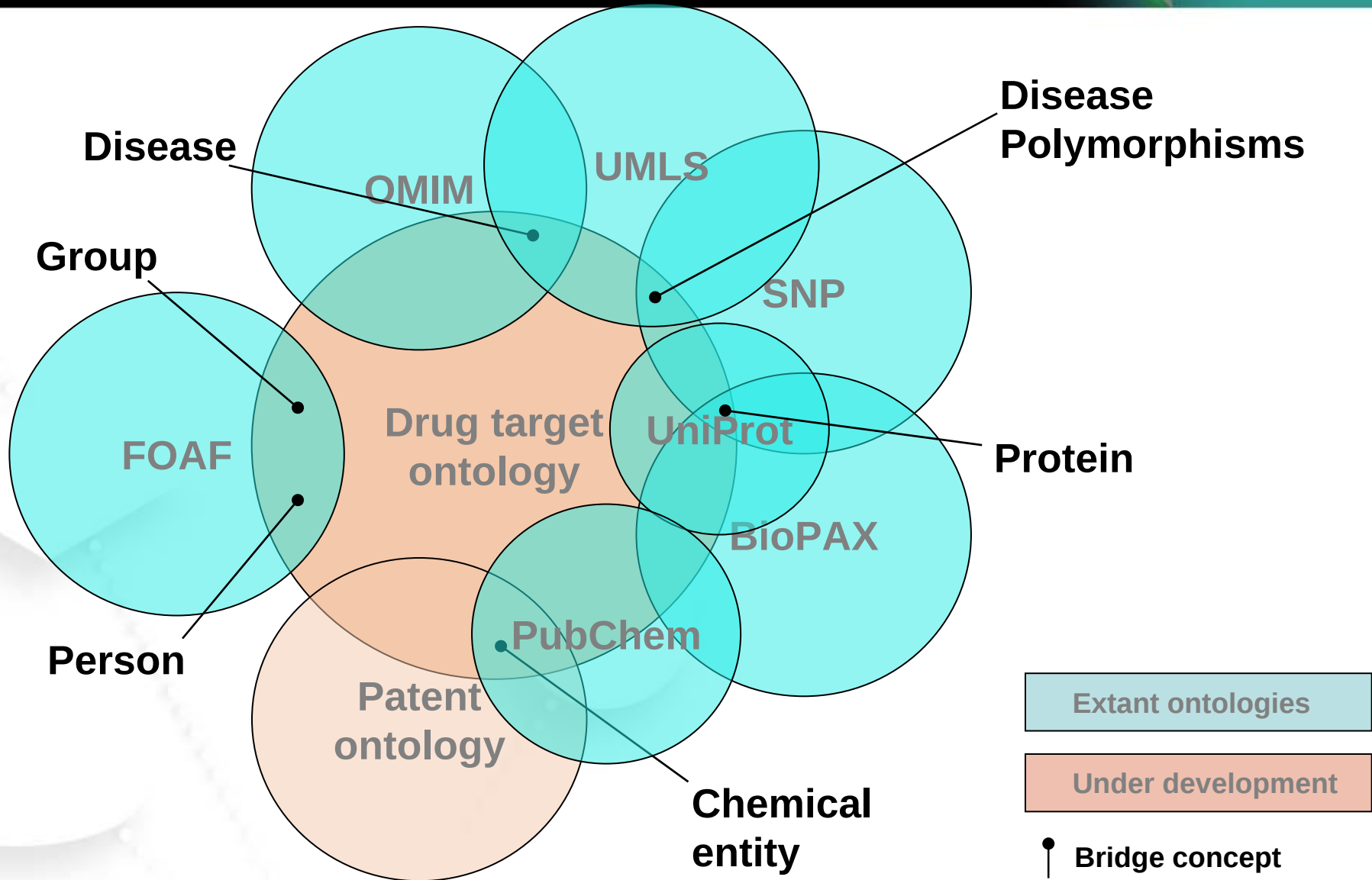


**Open Data Format and Flexible Linking Enables
Data Integration and Collaboration**

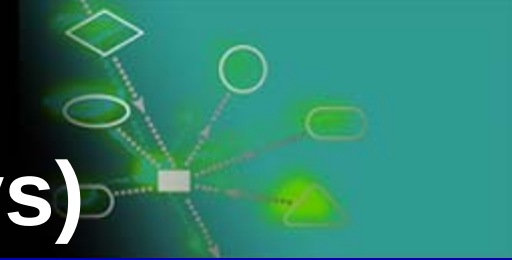
Semantic Web Drug DD Application Space



Multiple Ontologies Used Together



Case Study: BioPAX (Pathways)



QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.

```
<bp:PATHWAYSTEP rdf:ID="xDshToXGSK3bPathwayStep">
  <bp:next-step rdf:resource="#xGSK3bToBetaCateninPathwayStep"/>
  <bp:step-interactions>
    <bp:MODULATION rdf:ID="xDshToXGSK3b">
      <bp:keft rdf:resource="#xDsh"/>
      <bp:right rdf:resource="#xGSK-3beta"/>
      <bp:participants rdf:resource="#xGSK-3beta"/>
      <bp:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string">
        Dishevelled to GSK3beta</bp:name>
      <bp:direction rdf:datatype="http://www.w3.org/2001/XMLSchema#string">
        IRREVERSIBLE-LEFT-TO-RIGHT</bp:direction>
      <bp:control-type rdf:datatype="http://www.w3.org/2001/XMLSchema#string">
        INHIBITION</bp:control-type>
      <bp:participants rdf:resource="#xDsh"/>
    </bp:MODULATION>
  </bp:step-interactions>
</bp:PATHWAYSTEP>
```

Case Study: NeuroCommons.org

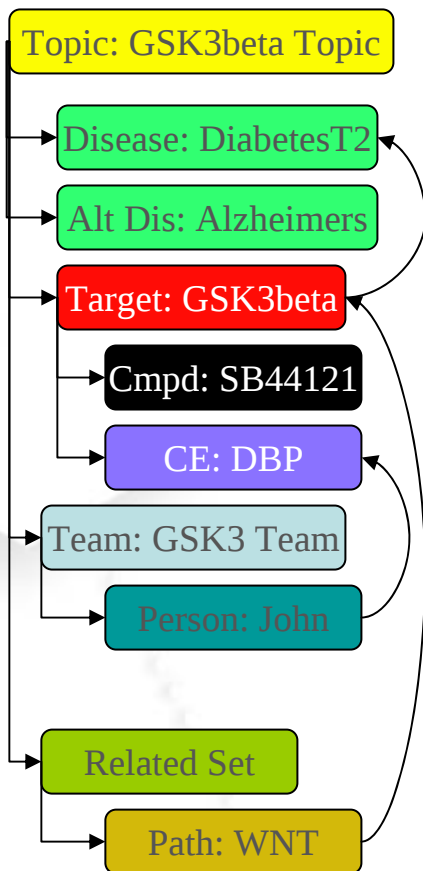


A collaboration between Science Commons and the Teranode Corporation, to create a free, public Semantic Web for neurological research.

1. To demonstrate that scientific impact and innovation is directly related to the freedom to legally reuse and technically transform scientific information.
2. To establish a legal and technical framework that increases the impact of investment in neurological research in a public and clearly measurable manner.
3. To develop an open community of neuroscientists, funders of neurological research, technologists, physicians, and patients to extend the NeuroCommons work in an open, collaborative, distributed manner.

Case Study: Drug Discovery Dashboard

<http://www.w3.org/2005/04/swls/BioDash>



The screenshot shows the Haystack application window. The title bar includes 'Project Haystack Run Window Help'. The main content area is titled 'GSK3beta Topic'. Below this, there are three sections: 'Target overview', 'Group members', and 'Primary disease'. The 'Target overview' section shows a diagram with several nodes (DBP Lead, SB..., A..., CHI..., AKAPaulic NCE, CHI...) all pointing to a central red box labeled 'GSK3beta'. The 'Group members' section contains a table with columns: Title, role, Department, and E-mail. The 'Primary disease' section shows 'Type 2 Diabetes' with a list of alternative titles and symbols, including 'DIABETES MELLITUS, NONINSULIN-DEPENDENT; NIDDM' and 'DIABETES MELLITUS, TYPE II NONINSULIN-DEPENDENT DIABETES MELLITUS'. It also includes a 'Gene map locus' section with the text '20q12-q13.1, 20q12-q13.1'.

GSK3beta Topic

Target overview

Diagram showing targets pointing to GSK3beta:

- DBP Lead
- SB...
- A...
- CHI...
- AKAPaulic NCE
- CHI...

Group members

Title	role	Department	E-mail
John Tegler	Medicinal Chemist	Chemistry	john.tegler
Steve Smith	Synthetic Chemist	Chemistry	steve.smit
Tim Gross	Molecular Modeler	Cheminformatics	tim.gross

Primary disease

Type 2 Diabetes

#125853 [Links](#)

DIABETES MELLITUS, NONINSULIN-DEPENDENT; NIDDM

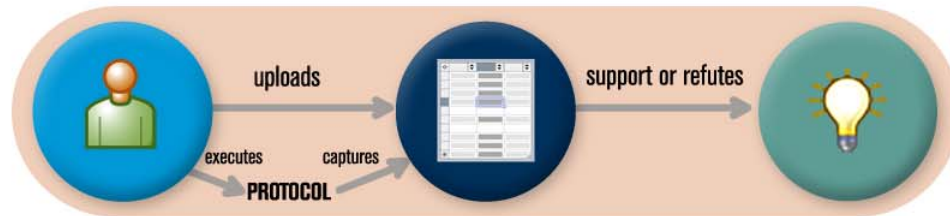
Alternative titles; symbols

DIABETES MELLITUS, TYPE II
NONINSULIN-DEPENDENT DIABETES
MELLITUS
MATURITY-ONSET DIABETES
INSULIN RESISTANCE, SUSCEPTIBILITY
TO, INCLUDED

Gene map locus [20q12-q13.1, 20q12-q13.1](#)

R&D Support

Scientist Creates Dataset to Test Hypothesis



R&D Support

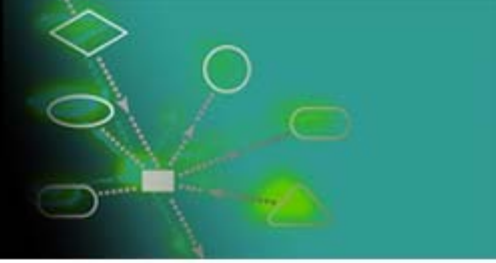


W3C Launches Semantic Web for HealthCare and Life Sciences Interest Group



- Interest Group formally launched Nov 2005:
<http://www.w3.org/2001/sw/hcls>
- First Domain Group for W3C - “...take SW through its paces”
- An Open Scientific Forum for Discussing, Capturing, and Showcasing Best Practices
- Recent life science members: Pfizer, Merck, Partners HealthCare, CSIRO, Teranode, Cerebra, NIST, U Manchester, Stanford U, AlzForum, Oracle, IBM, HP, Siemens, AGFA
- Co-chairs:
 - Dr. Tonya Hongsermeier (Partners HealthCare)
 - Eric Neumann (Teranode)

Current HCLS Activities



- BioRDF - data as RDF (structured and NLP)
- BioONT - ontology coordination
- Scientific Publishing - evidence management
- Adaptive Healthcare Protocols



Efficiency and Innovation: Semantic Web Applications Roadmap