Progress Towards an Ontology Mapping Service

Ian Harrow¹, Ernesto Jimenez-Ruiz², Thomas Liener³, Simon Jupp³
and The Ontologies Mapping Project¹

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SWAT4LS on 5th Dec 2018 in Antwerp
Outline

1. Pistoia Alliance
2. Application of Ontologies and Mappings
3. Progress Towards an Service
About Pistoia Alliance

Mission
• A global not-for-profit alliance of life science companies, vendors, publishers and academic groups
  – Lowering the barriers to innovation in Life Sciences R & D
  – [www.pistoiaalliance.org](http://www.pistoiaalliance.org) for more information

Business value
• Precompetitive research brings value through...
  – Building new standards, tools and services
  – Sharing best practice with industry peers
  – Evaluation of tools and services
  – And much more....
Project portfolio pipeline

Active Portfolio
- Ontologies Mapping
- Chemical Safety Library
- Macromolecule Notation
- Controlled Substance Compliance
- User Experience in Life Sciences (UXLS)
- Antibody 3D structures in the PDB
- Unified chemistry data model

Developing Portfolio
- Faster Companion Diagnostics in the Regulatory Domain
- Blockchain
- AI Centre of Excellence for Life Science R&D
- Laboratory of the Future
- FAIR data management
Outline

1. Pistoia Alliance

2. Application of Ontologies and Mappings

3. Progress Towards an Service
Ontology Features: Example from Gene Ontology

1) Class Terms (Controlled Vocabulary or TBox)

Class: (+)-2-epi-prezizaene synthase activity

Term IRI: http://purl.obolibrary.org/obo/GO_0102201
Definition: Catalysis of the reaction: 2-cis,6-trans-farnesyl diphosphate ↔ (+)-2-epi-prezizaene + diphosphoric acid

Annotations
- database_cross_reference:MetaCyc:RXN-12117 (= ontology mapping)
- has_oobo_namespace:molecular_function
- id:GO:0102201

2) Class Hierarchy (Structure or ABox)

Class Hierarchy

Thing
+ molecular_function
  + catalytic_activity
    + lyase_activity
      + carbon-oxygen lyase activity
        + carbon-oxygen lyase activity, acting on phosphates
          - 3-dehydroquinate synthase activity
          - 6-phospho-D-gluconate synthase activity
          - chorismate synthase activity
          - threonine synthase activity
          - betaine dehydrogenase activity
          + terpene synthase activity
          - germanium synthase activity
          - S-linalool synthase activity
          - R-linalool synthase activity
          - ent-cassia-12,15-diene synthase activity
          - stemar-13-ene synthase activity
          - syn-pimara-7,15-diene synthase activity
          more...
        - (+)-2-epi-prezizaene synthase activity

3) Identifier

Source: http://www.ontobee.org
What is Ontologies Mapping?

Data domain Example: Disease and Phenotype

Ontology 1 ➔ Ontology 2 ➔ Ontology 3

Expandable coverage

Mapping Tools and Services

⇒ Highly scalable and much more maintainable
⇒ A better engineering solution for application ontologies

+ More...
Application of ontologies and mappings

- Pharma executives now consider data as a valuable corporate assets to enable digital transformation
  - Data integration throughout an enterprise e.g. Horizontal Terminology Services
- Data Technology companies bridge the gap between “big data” and “innovative biological insight”
  - Data curation, valuation and governance
  - E.g. Eaglecore knowledge management platform at Roche
- Semantic analytics companies harness unstructured data
  - Data extraction and building knowledge with text mining
  - E.g. SciBite and Linguamatics platforms

Ontologies and mappings bring structure to linked data stores
Outline

1. Pistoia Alliance

2. Application of Ontologies and Mappings

3. Progress Towards an ONTOLOGIES MAPPING Service
3. The Ontologies Mapping Challenge

- Ontologies can include hierarchical relationships; taxonomies; classifications and vocabularies.
- They underpin numerous applications such as semantic search, linked data integration and text mining.
- Ontologies are the “smart glue” of linked data to semantically enable knowledge management.

**BUT...**

- Ontologies and their mappings are very costly to curate.
- Many varying ontologies overlap in the **same data domain** e.g. disease and phenotype.
- Need better practice, tools and services to manage and apply ontologies, including **how they map to each other**.

**The Ontologies Mapping Project**
Ontologies Mapping Project Overview

Pistoia Members

OM Project

Outputs: 1) Guidelines for best practice, 2) evaluation of tools & 3) prototype service

Community of Interest

Agri-food

Academics

Individuals

Pharmaceuticals

Technology providers

Publishers

OM Project Team

Funders
Guidelines for Selection of Ontologies

<table>
<thead>
<tr>
<th>Guideline:</th>
<th>Ontology:</th>
<th>Human Disease ontology (DOID)</th>
<th>Human Phenotype (HPO)</th>
<th>Mammalian Phenotype (MP)</th>
<th>Clinical Terms SNOMED-CT</th>
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<td>Okay</td>
<td>Okay</td>
<td>Okay</td>
<td>Okay (mostly!)</td>
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- These guidelines are accessible from a public wiki: - https://pistoiaalliance.atlassian.net/wiki/display/PUB/Ontologies+Mapping+Resources
- They align with the principles found at the OBO Foundry: - http://www.obofoundry.org
Ontologies Mapping Tool Overview

User Interface
- Visualisation of ontological space
- Mapping Alignment Editor

Framework
- Workflow and Evaluation
- Ontology Matching algorithms

Detailed requirements are available on the OM project public wiki: https://pistoiaalliance.atlassian.net/wiki/display/PUB/Ontologies+Mapping+Resources
## Tool Requirements & Evaluation of Capability

### Functional Requirements

<table>
<thead>
<tr>
<th>Requirement</th>
<th>Academic 1</th>
<th>Academic 2</th>
<th>Academic 3</th>
<th>Commercial 2</th>
<th>Commercial 1</th>
<th>Academic 4</th>
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### None-Functional requirements

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<th>Academic 2</th>
<th>Academic 3</th>
<th>Commercial 2</th>
<th>Commercial 1</th>
<th>Academic 4</th>
<th>Commercial 3</th>
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<td>1. No License restrictions for use</td>
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<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
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<td>2. Current Availability &amp; Maintenance</td>
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<td>2</td>
<td>2</td>
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<td>3. Standalone and web service</td>
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<td>2</td>
<td>1</td>
<td>2</td>
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</table>

Key:
- **Yes** = 2
- **Partial** = 1
- **Expected** = 0
- **No** = 0

LogMap, AML, OLS/OXO, YAM++, Mondeca, Infotech, fluidOps

Detailed requirements and results are available on the OM project public wiki: [https://pistoiaalliance.atlassian.net/wiki/display/PUB/Ontologies+Mapping+Resources](https://pistoiaalliance.atlassian.net/wiki/display/PUB/Ontologies+Mapping+Resources)
Ontology Alignment Evaluation Initiative
http://oaei.ontologymatching.org

• 2016 Campaign – publication on phenotype track

• Numerous tracks include one for Disease and Phenotype
  – Pistoia Alliance Ontologies Mapping project organise 2 mapping tasks:
    • Human Phenotype (HP) Ontology vs. Mammalian Phenotype (MP) Ontology
    • Human Disease Ontology (DOID) vs. Orphanet & Rare Diseases Ontology (ORDO)

• Phenotype track repeated for 2017 and 2018 Campaigns
  – ~50% of ~20 participating systems completed either or both tasks
  – Consistent top performing systems: AML and LogMap
### Top performers for OAEI 2017 in phenotype track

<table>
<thead>
<tr>
<th>OM algorithm</th>
<th>Track Task</th>
<th>Total Equivalence Mappings</th>
<th>Precision Silver 3 Equiv mappings</th>
<th>Recall Silver 3 Equiv mappings</th>
<th>F-Score Silver 3 Equiv mappings</th>
<th>Sum F Scores Silver 3 Equiv mappings</th>
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<td>AML</td>
<td>HP-MP</td>
<td>2029</td>
<td>0.822</td>
<td>0.951</td>
<td>0.882</td>
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<td>HP-MESH</td>
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<td>0.677</td>
<td>0.805</td>
<td>0.992</td>
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<td>0.624</td>
<td>0.768</td>
<td>0.998</td>
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<td>HP-MP</td>
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<td>0.500</td>
<td>0.678</td>
<td>0.576</td>
<td>3.144</td>
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<td>0.603</td>
<td>0.684</td>
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<td>0.649</td>
<td>0.518</td>
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<td>0.672</td>
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<td>0.941</td>
<td>0.895</td>
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Source: This data is from the 3 vote consensus
Ontologies at EMBL-EBI

Biomedical ontologies

- Gene function
- Phenotype
- Disease
- Plant anatomy
- Cell types
- Taxonomy
- Cell lines
- Small molecules
- BioAssays
- Evidence
- Mouse anatomy
- Information
- Drugs
- Adverse events

Applications

- BioSamples
- EBiSC
- ENA
- EVA
- Expression Atlas
- GWAS catalog
- Open Targets
- UniProt
- QuickGO
- Array Express
- ClinVar

Source: Dr Simon Jupp (EMBL-EBI)
Building an Ontology Toolkit and Services

- **Ontology Lookup Service (OLS)**: Search/Visualise ontologies
- **Zooma**: Annotate data
- **OxO**: Ontology Mappings
- **Webulous**: Create new ontology content

Source: Dr Simon Jupp (EMBL-EBI)  
Grants: ELIXIR-EXCELERATE 676559 & CORBEL 654248
• Collaborate with EMBL-EBI to build on their existing services
• Develop a new algorithm to predict mappings between any two ontologies
Relationship between OxO mapping repository and the new mapping algorithm, Paxo

Prototype Ontology Mapping Service

<table>
<thead>
<tr>
<th>10 ontology mappings</th>
<th></th>
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<tbody>
<tr>
<td>HP-DOID</td>
<td>MeSH-ORDO</td>
</tr>
<tr>
<td>HP-ORDO</td>
<td>MP-HP</td>
</tr>
<tr>
<td>DOID-ORDO</td>
<td>MP-DOID</td>
</tr>
<tr>
<td>MeSH-HP</td>
<td>MP-ORDO</td>
</tr>
<tr>
<td>MeSH-DOID</td>
<td>MeSH-MP</td>
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</table>
OxO Ontology Mappings Service

List of Identifiers Or labels

Export mapping

1,540 matches

Human Disease Ontology

Orphanet
Optimisation of the predicted ontology mappings for unique matches: evaluation of quality

<table>
<thead>
<tr>
<th>Mapping</th>
<th>Predicted matches total</th>
<th>Predicted in silver</th>
<th>Silver standard</th>
<th>Missed matches</th>
<th>Recall</th>
<th>Additional matches</th>
<th>Precision for additions (N=60)</th>
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<td>12</td>
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</tbody>
</table>

Silver standard is a consensus from a panel of ontology mapping algorithms from OAEI2017
Optimisation of the predicted ontology mappings for multiple matches: evaluation of quality

<table>
<thead>
<tr>
<th>Mapping</th>
<th>Predicted matches total</th>
<th>Predicted in silver</th>
<th>Silver standard</th>
<th>Missed matches</th>
<th>Recall</th>
<th>Additional matches</th>
<th>Precision for additions (N=60)</th>
</tr>
</thead>
<tbody>
<tr>
<td>mesh_mp</td>
<td>868</td>
<td>282</td>
<td>282</td>
<td>0</td>
<td>100.00%</td>
<td>586</td>
<td>88.30%</td>
</tr>
<tr>
<td>mesh_doid</td>
<td>2280</td>
<td>1261</td>
<td>1265</td>
<td>4</td>
<td>99.68%</td>
<td>1019</td>
<td>81.70%</td>
</tr>
<tr>
<td>mesh_hp</td>
<td>1519</td>
<td>728</td>
<td>734</td>
<td>6</td>
<td>99.18%</td>
<td>791</td>
<td>60.00%</td>
</tr>
<tr>
<td>hp_doid</td>
<td>3636</td>
<td>1156</td>
<td>1348</td>
<td>192</td>
<td>85.76%</td>
<td>2480</td>
<td>40.00%</td>
</tr>
<tr>
<td>ordo_doid</td>
<td>5375</td>
<td>2178</td>
<td>2553</td>
<td>375</td>
<td>85.31%</td>
<td>3197</td>
<td>73.30%</td>
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<tr>
<td>ordo_hp</td>
<td>2382</td>
<td>623</td>
<td>767</td>
<td>144</td>
<td>81.23%</td>
<td>1759</td>
<td>68.30%</td>
</tr>
<tr>
<td>ordo_mesh</td>
<td>1079</td>
<td>632</td>
<td>782</td>
<td>150</td>
<td>80.82%</td>
<td>447</td>
<td>88.30%</td>
</tr>
<tr>
<td>ordo_mp</td>
<td>958</td>
<td>141</td>
<td>185</td>
<td>44</td>
<td>76.22%</td>
<td>817</td>
<td>56.70%</td>
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<tr>
<td>mp_doid</td>
<td>2473</td>
<td>320</td>
<td>465</td>
<td>145</td>
<td>68.82%</td>
<td>2153</td>
<td>30.00%</td>
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<tr>
<td>mp_hp</td>
<td>7190</td>
<td>1446</td>
<td>2128</td>
<td>682</td>
<td>67.95%</td>
<td>5744</td>
<td>43.30%</td>
</tr>
</tbody>
</table>

Silver standard is a consensus from a panel of ontology mapping algorithms from OAEI2017
Summary

• Guidelines to select ontologies prior to application
• Requirements vs. capabilities of commercial and academic mapping tools
• Phenotype track for OAEI challenge to determine top performing algorithms
• Progress towards a prototype Ontology Mapping Service

Significance

• Predicted Ontology Mappings from algorithms and validated by manual curation gives extended their coverage across a domain to support semantically-enabled applications

Plan for Next Phase

• Build Ontology Mappings to support biology and chemistry lab data analytics
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- Accenture (3)
- Bayer (3)
- Merck & Co (1,2)
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Project team
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