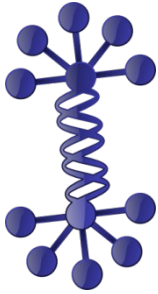


Analysis and visualisation of RDF resources in Oindex

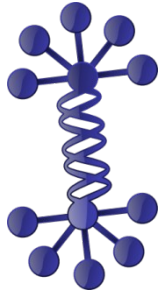
Catherine Canevet

catherine.canevet@bbsrc.ac.uk



Motivation

- Biomedical resources provide info on the Semantic Web
- Potential to advance biomedical research
- Need for tools
 - Data reduction
 - Data visualization
 - Interactive analysis capabilities

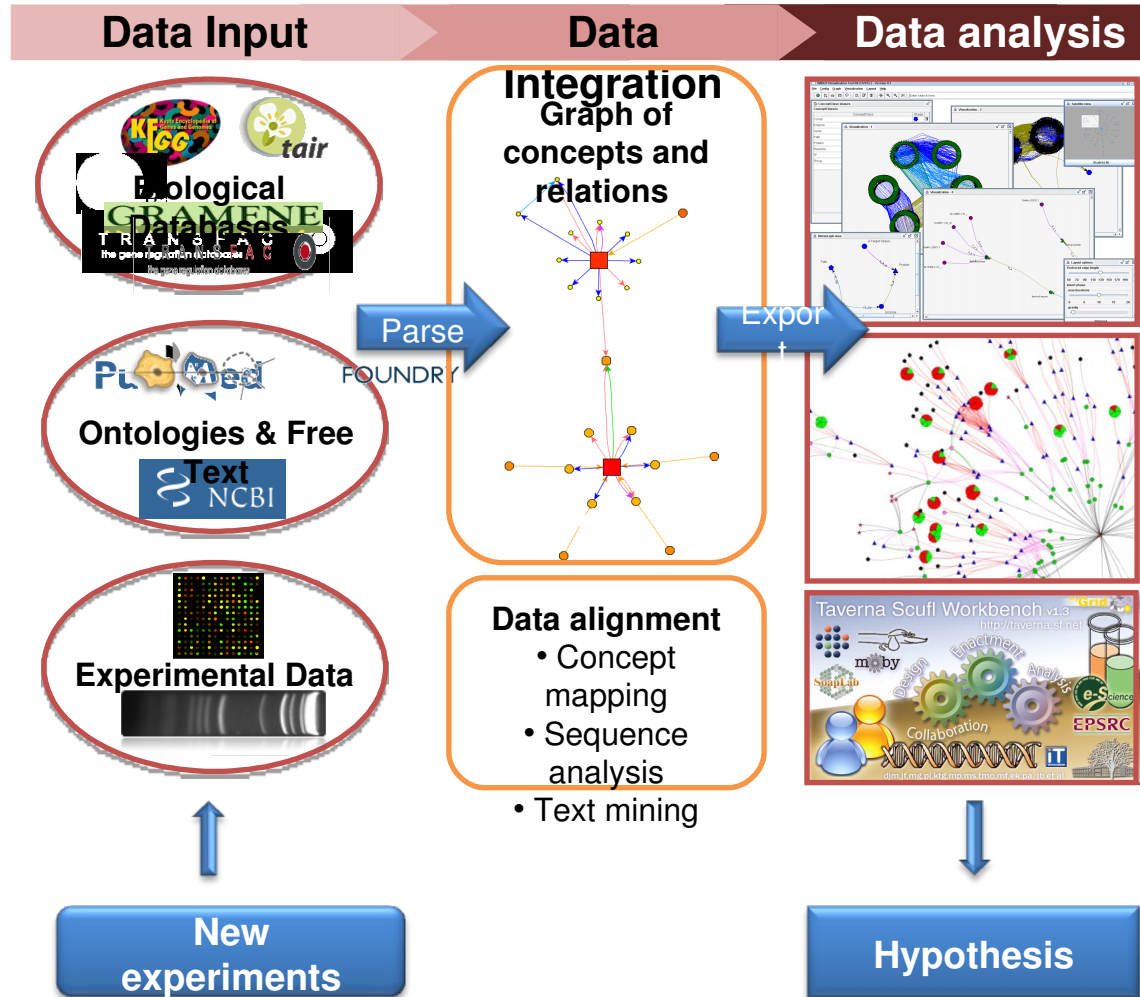


Ondex: a platform to exploit the Semantic Web

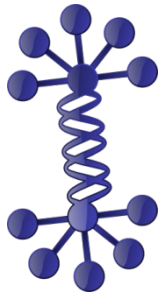
- 1) all information can be represented as a graph
- 2) all elements of the graph can be annotated with ontologies
- 3) data model conformant to Semantic Web framework, in particular to RDF

➔ Ondex ideally positioned

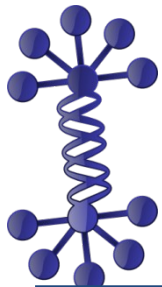
Data integration and visualisation in Ondex



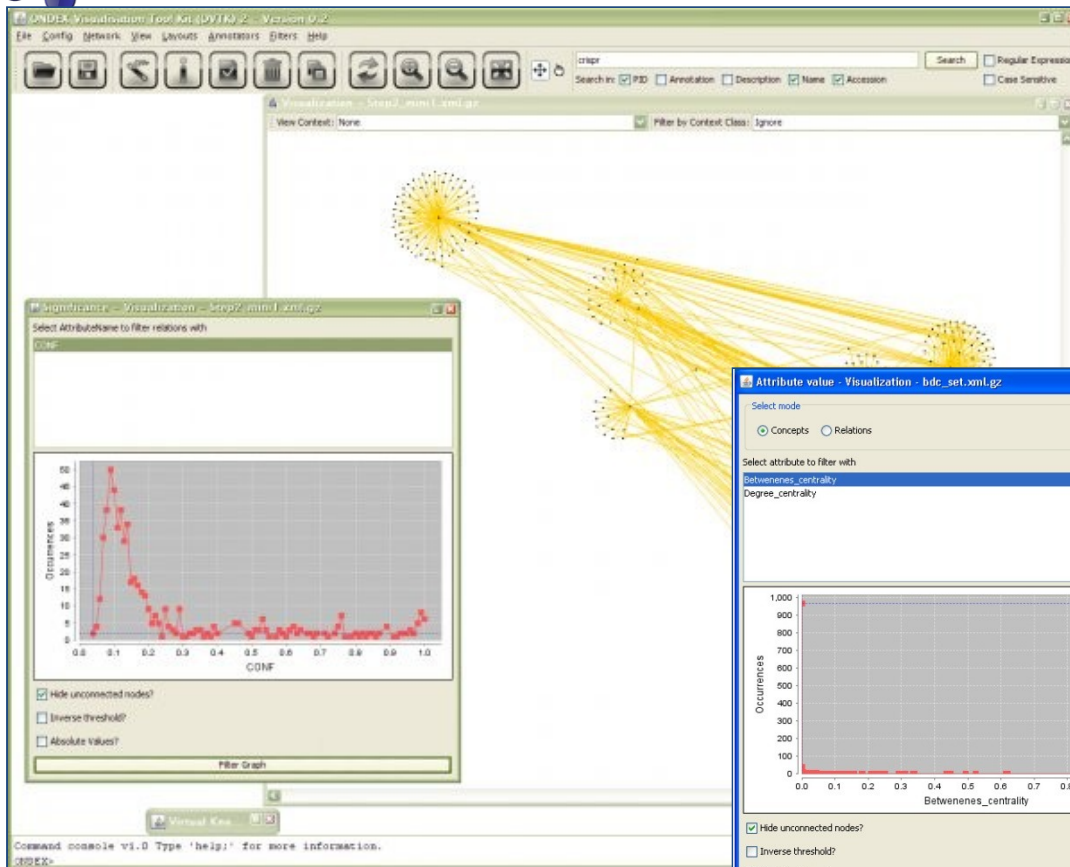
Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010



Data reduction and representation methods

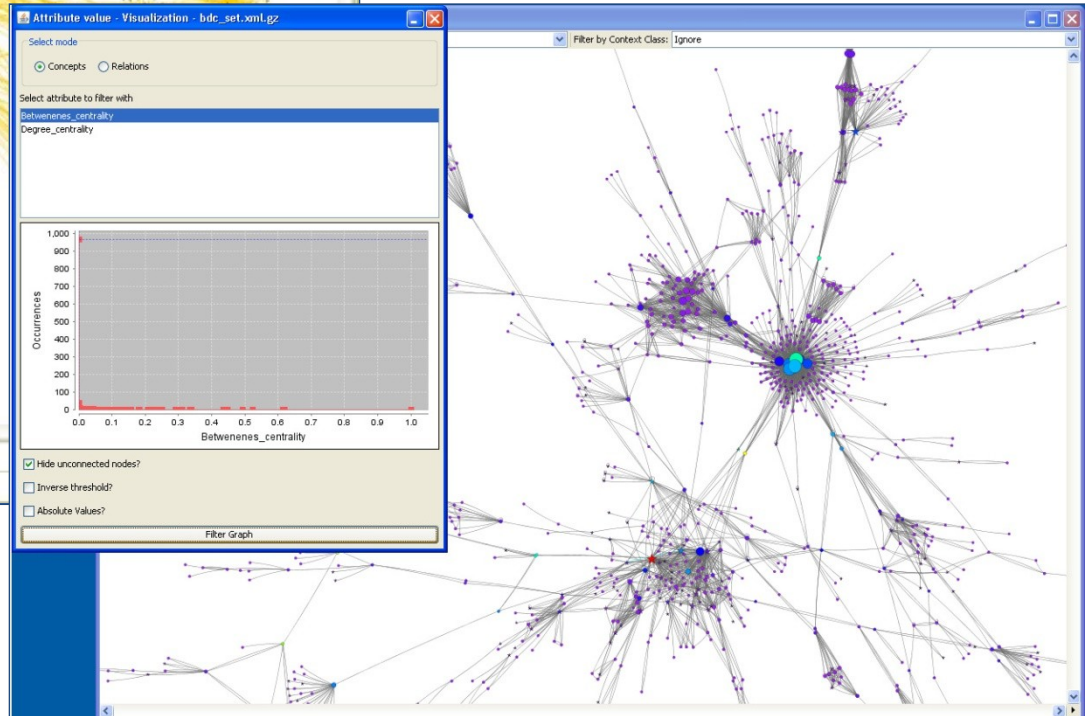


Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010



Filter on confidence

Filter on centrality



- Export
 - Experimental
 - Discontinued
 - Stable
 - OXL Export
 - Report writer
- Filter
 - Discontinued
 - Stable
 - Experimental
 - Graph
 - Mapping
 - Stable
 - Concept accession-based mapping (Memory-efficient)
 - Inparanoid
 - Experimental
 - Parser
 - Stable
 - Aracyc2 (Release 6, October 14, 209)
 - BCSDB (pre-release BCSDB-3 gamma version)
 - Brenda specific SBML Parser (BRENDA release online since 2nd July 2010)
 - EXPASY ENZYME (4/10/2009)
 - FASTA file parser
 - KEGG parser (Release 52.1, December 1, 2009)
 - KEGG parser, latest (Release 53.0, January 1, 2010)
 - OXL Parser
 - UniProt (UniProt release July2010)
 - Experimental
 - Statistics
 - Experimental
 - Transformer
 - Experimental
 - Stable
 - Relation Collapser

Arguments | Documentation | Required data | Comments

a subset of the TAIR9 database parsing genes, proteins, domains

Annotation If true also GO annotations, protein domain information and UniProt accessions will be parsed

InputDir Absolute path to input directory

Graph id Graph that will be operated on by this plugin.

New

New memory graph

GraphName default
Graph id default

TAIR 9

Annotation
InputDir
Graph id default

UniProt

InputDir
TaxId
DbRefAcc
Accessions
AccessionsFile
ContextInformation
HideLargeScaleRef
GoFile
Graph id default

Concept accession-based mapping (Memory-efficient)

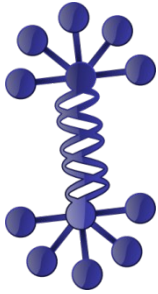
EquivalentCC
EquivalentCV
GDSEqualsConstraint
IgnoreAmbiguity
RelationType equ
WithinCVMMapping
ConceptClassRestriction
CVRrestriction
Graph id default

Relation Collapser

RelationType
ConceptClassRestriction
CVRrestriction
CloneGDS
CreateGDSsets
Graph id default

OXL Export

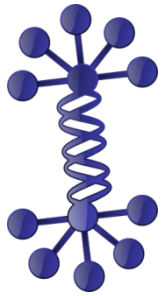
ExcludeConceptsOfConceptClass
ExcludeRelationsOfRelationType
ExcludeGDSWithAttribute
IncludeOnlyGDSAttribute
IncludeOnlyConceptClass
IncludeOnlyRelationType
Pretty
ExportIsolatedConcepts
GZip
FormatFile



Demo

- Interactive importer based on SPARQL
- Query-driven construction of datasets
- Bring information from different RDF data resources into Oindex
- Welcome feedback on our prototype

Data used in demo integrated by Keywan Hassani-Pak



Input

45778 predicted poplar genes

Data Integration

PoplarCyc, Poplar TFDB

Comparative Genomics

BLAST against UniProt Plants

HMMer against Pfam

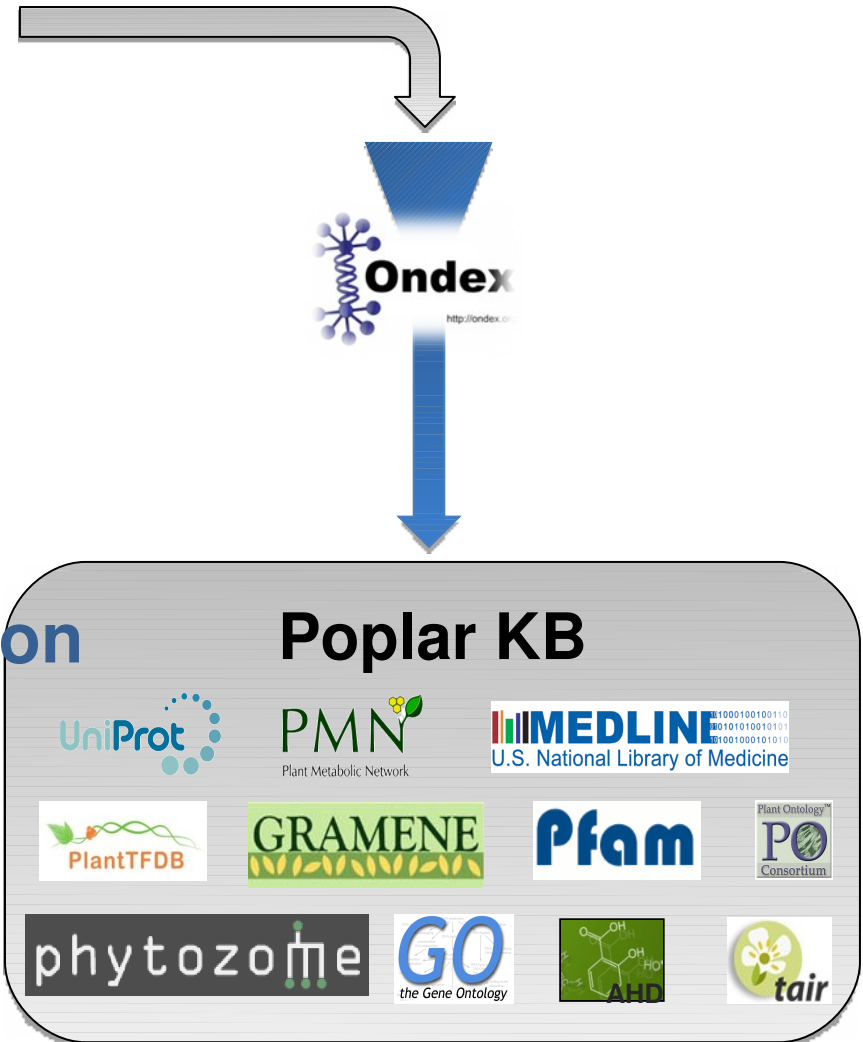
Inparanoid to Arabidopsis

Autom. Function Prediction

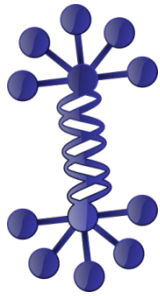
Gene, Plant and Trait Ontology

Text Mining

Co-occurrence of genes and traits in Medline abstracts



Connecting and querying



Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010

The screenshot shows the Ondex software interface. The main window is titled "Ondex - Version 0.3 (build null)". The menu bar includes File, Edit, View, Appearance, Tools, and Help. The toolbar contains various icons for file operations and search. The search bar contains the text "Enter search here...". The search results are displayed in a table with columns for Name, Parser ID, Type, DataSource, and Evidence. The search results are:

Name	Parser ID	Type	DataSource	Evidence
http://www.ondex.org/concept/313	http://www.ondex.org/concept/313	TO	http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql	IMPD

The "Item Information" window shows the following details for the selected item:

General Information
Name: <http://www.ondex.org/concept/313>
Parser ID: <http://www.ondex.org/concept/313>
Type: TO
DataSource: <http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql>
Evidence: IMPD

Tags

Synonyms
<http://www.ondex.org/concept/313>
shoot branching

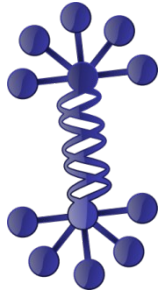
Accessions

URI
<http://www.ondex.org/concept/313>

The "Console" window shows the following commands and output:

```
Command console v1.0 Type 'help;' for more information.
ONDEX>sparql_mode
Changing configuration - please wait...
SPARQL interpreter loaded successfully
ONDEX>connect("http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql")
ONDEX>construct {?x ?y "shoot branching"}
where {graph ?g (?x ?y "shoot branching")}
ONDEX>
```

Right-click pre-defined queries



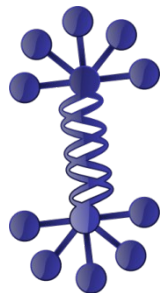
Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010

The screenshot displays the Ondex software interface, version 0.3 (build null). The main window is titled "Ondex - Version 0.3 (build null)" and contains several panes:

- Item Information:** A pane on the left showing details for a concept. It includes sections for General Information (Name, Parser ID, Type, DataSource, Evidence), Tags, Synonyms, Accessions, and URI.
- Visualization - 0:** A large central area for visualizing data. A right-click context menu is open over this area, showing options: Link, Hide, Show, Show / Edit Properties, and Query. The Query option is expanded, showing sub-options: Find relations subjects of, Find relations objects of, Find subjects of, Fill attributes, Find objects of, and Resolve URL.
- Console:** A pane at the bottom showing the command-line interface. It displays the following text:

```
Command console v1.0 Type 'help;' for more information.
ONDEX>sparql_mode
Changing configuration - please wait...
SPARQL interpreter loaded successfully
ONDEX>connect ("http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql")
ONDEX>construct {?x ?y "shoot branching"}
where {graph ?g {?x ?y "shoot branching"}}
ONDEX>
```

Filling attributes



Ondex - Version 0.3 (build null)

File Edit View Appearance Tools Help

Enter search here... Regular Expr. Case Sensitive

Restrict by: Concept Class Data Source Tag

Item Information

View

General Information

Name: <http://www.ondex.org/concept/292>
Parser ID: 13130077
Type: Publication
DataSource: <http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql>
Evidence: IMPD

Annotation

[NUCLEOTIDE SEQUENCE [MRNA], FUNCTION, TISSUE SPECIFICITY, DEVELOPMENTAL STAGE, MUTAGENESIS OF ALA-49 AND ARG-50]

Tags

Synonyms

<http://www.ondex.org/concept/292>
PMID:13130077

Accessions

<http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql:10.1073/PNAS.1932414100> 13130077

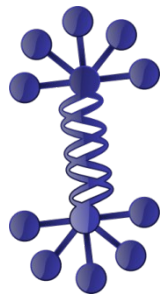
Publication

LAX and SPA: major regulators of shoot branching in rice.
Keishi Komatsu, Masahiko Maekawa, Shin Ujiie, Yuzuki Satake, Ikuyo Furutani, Hironobu Okamoto, Ko Shimamoto, Junko Kyoizuka
Year: 2003
Published in: Proc. Natl. Acad. Sci. U.S.A.
The aerial architecture of plants is determined primarily by the pattern of shoot branching. Although shoot apical meristem initiation during embryogenesis has been extensively studied by molecular genetic approaches using Arabidopsis, little is known about the genetic mechanisms controlling axillary meristem initiation, mainly because of the insufficient number of mutants that specifically alter it. We identified the LAX PANICLE (LAX) and SMALL PANICLE (SPA) genes as the main regulators of axillary meristem formation in rice. LAX encodes a basic helix-loop-helix transcription factor and is expressed in the boundary between the shoot apical meristem and the region of new meristem formation. This pattern of LAX expression was repeatedly observed in every axillary meristem, consistent with our observation that LAX is involved in the formation of all types of axillary meristems throughout the ontogeny of a rice plant. Ectopic LAX expression in rice caused pleiotropic effects, including dwarfing, an altered pattern of stem elongation, darker color, bending of the lamina joint, absence of the midribs of leaves, and severe sterility.

Visualization - 0

Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010

Proteins related to shoot branching



Oindex - Version 0.3 (build null)

File Edit View Appearance Tools Help

Enter search here... Regular Expr. Case Sensitive

Restrict by: Concept Class Data Source Tag

Item Information

View

General Information

Name: <http://www.ondex.org/concept/159>
Parser ID: LAX
Type: Protein
DataSource: <http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql>
Evidence: IMPD

Tags

Synonyms

<http://www.ondex.org/concept/159>
LAX
LAX1
LOC_Os01g61480
Os01g0831000
P0446G04.27
Transcription factor LAX PANICLE

Accessions

<http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql>: AP003252
G7XAG6 PS50888 IPR001092 AB115668 4327431
LOC_Os01g0831000 OSA:4327431 OS:38423 PF00010
NP_001044699.1 Os01g0831000

Taxonomy

[39947](#)

Aminoacid sequence (AA):

MDPFGFP I HPQYHLNPT AGLGGEMR
GGGRFRGAK LSTDPQVAA RERFRISDR
F PULRSLVP GGSMDTVSM LEQALHYWKT
LKAQVTLHQA ALVQNEEGCC HADVAARSA
AD ADLALQL MRRHGAGDD DAGHTLEMA
PHEQAVGYGD GPAAQHMQA LDFAGQLMGC

Visualization - 0

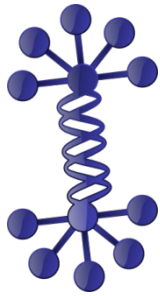
Metadata Legend

Concept Classes	Data Sources	RelationTypes	EvidenceTypes
		Publication 12 (12)	
		TO 7 (7)	
		Protein 8 (8)	
Total Concepts 27 (27)			
<input type="button" value="Copy to clipboard"/>			
<input type="button" value="Refresh Metadata"/>			

Console

```
Command console v1.0 Type 'help;' for more information.
ONDEX>sparql_mode
Changing configuration - please wait...
SPARQL interpreter loaded successfully
ONDEX>connect("http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql")
ONDEX>construct {?x ?y "shoot branching"}
where {graph ?g {?x ?y "shoot branching"}}
ONDEX>
```

Colour proteins by taxonomy ID



Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010

Oindex - Version 0.3 (build null)

File Edit View Appearance Tools Help

Enter search here... Regular Expr. Case Sensitive

Restrict by: Concept Class Data Source Tag

Colour Concepts by Gene...

Select attribute to annotate concepts with

- DOI
- JOURNAL_REF
- JOURNAL_REF:0
- MeSH
- PUB_TYPE
- TAXID**
- URI
- YEAR

Set blanks to white?

Exclusive use of attribute?

Annotate Graph

Legend Colour Con...

Color
3694
39947

Visualisation - 0

Network visualization showing concepts connected to a central node. Nodes are color-coded by taxonomy ID (TAXID).

Metadata Legend

Concept Classes	Data Sources	RelationTypes	EvidenceTypes
		Publication	12 (12)
		TO	7 (7)
		Protein	8 (8)
Total Concepts 27 (27)			

Copy to clipboard

Refresh Metadata

Console

```
Command console v1.0 Type 'help;' for more information.
ONDEX>sparql_mode
Changing configuration - please wait...
SPARQL interpreter loaded successfully
ONDEX>connect("http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql")
ONDEX>construct {?x ?y "shoot branching"}
where {graph ?g {?x ?y "shoot branching"}}
ONDEX>
```

Colour Concepts by Gene...

cept/159

msted.bbsrc.ac.uk:8050/sparql

9

LOC_Os01g01400
Os01g0831000
P0446G04.27
Transcription factor LAX PANICLE

Accessions

<http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql>: AP003252
G7XAG6 PS50888 IPR001092 AB115668 4327431
LOC_Os01g0831000 OSA:4327431 OS:38423 PF00010
NP_001044699.1 Os01g0831000

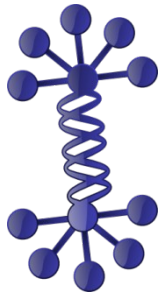
Taxonomy

[39947](http://www.ncbi.nlm.nih.gov/tx/39947)

Aminoacid sequence (AA):

```
MDPFGFP I HPQYHLNPT AGLGEGMR  
GGGRFPGAK LSTDPQSVAA RERHRISDR  
F PULRSLVP GGSMDTVSM LEQIHYVKT  
LKAQVTLHQA ALVQNEEGCQ HADVAATSA  
AD ADLALEL MRRHGAGDD DAGHTLEMA  
PHEAUGYGD GPARQHQQA LDFAGQLHGC
```

Scale relation based on BLAST



Nature Precedings : doi:10.1038/npre.2010.5430.1 : Posted 23 Dec 2010

The screenshot displays the Ondex software interface, Version 0.3 (build null). The main window shows a network visualization of concepts and their relationships. The concepts are represented by nodes (squares and triangles) connected by edges (lines). The nodes are color-coded based on their relationships, with a legend provided in the 'Legend Colour Con...' window. The nodes are labeled with URIs such as <http://www.ondex.org/concept/317>, <http://www.ondex.org/concept/313>, <http://www.ondex.org/concept/315>, <http://www.ondex.org/concept/319>, <http://www.ondex.org/concept/307>, <http://www.ondex.org/concept/316>, <http://www.ondex.org/concept/318>, <http://www.ondex.org/concept/314>, <http://www.ondex.org/concept/324>, <http://www.ondex.org/concept/328>, <http://www.ondex.org/concept/294>, <http://www.ondex.org/concept/298>, <http://www.ondex.org/concept/296>, <http://www.ondex.org/concept/299>, <http://www.ondex.org/concept/312>, <http://www.ondex.org/concept/298>, <http://www.ondex.org/concept/320>, <http://www.ondex.org/concept/293>, <http://www.ondex.org/concept/297>, <http://www.ondex.org/concept/295>, <http://www.ondex.org/concept/292>, <http://www.ondex.org/concept/291>, <http://www.ondex.org/concept/290>, <http://www.ondex.org/concept/289>, <http://www.ondex.org/concept/287>, <http://www.ondex.org/concept/285>, 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<http://www.ondex.org/concept/65>, <http://www.ondex.org/concept/63>, <http://www.ondex.org/concept/61>, <http://www.ondex.org/concept/59>, <http://www.ondex.org/concept/57>, <http://www.ondex.org/concept/55>, <http://www.ondex.org/concept/53>, <http://www.ondex.org/concept/51>, <http://www.ondex.org/concept/49>, <http://www.ondex.org/concept/47>, <http://www.ondex.org/concept/45>, <http://www.ondex.org/concept/43>, <http://www.ondex.org/concept/41>, <http://www.ondex.org/concept/39>, <http://www.ondex.org/concept/37>, <http://www.ondex.org/concept/35>, <http://www.ondex.org/concept/33>, <http://www.ondex.org/concept/31>, <http://www.ondex.org/concept/29>, <http://www.ondex.org/concept/27>, <http://www.ondex.org/concept/25>, <http://www.ondex.org/concept/23>, <http://www.ondex.org/concept/21>, <http://www.ondex.org/concept/19>, <http://www.ondex.org/concept/17>, <http://www.ondex.org/concept/15>, <http://www.ondex.org/concept/13>, <http://www.ondex.org/concept/11>, <http://www.ondex.org/concept/9>, <http://www.ondex.org/concept/7>, <http://www.ondex.org/concept/5>, <http://www.ondex.org/concept/3>, <http://www.ondex.org/concept/1>.

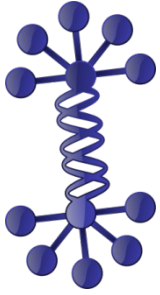
The interface includes several panels:

- Scale/Colour Relations by N...:** Contains options for 'resize relations' (Min Relation Size: 1, Max Relation Size: 10), 'inverse scaling', 'colour edges', and 'Min Colour' (blue, red, black). It also lists attributes for annotation: BITSCORE, BLEV, COVERAGE, OVERLAP, QUERY_LENGTH, TARGET_LENGTH, TRANSLATION_FRAME.
- Legend Colour Con...:** A table showing the mapping of concept IDs to colors.
- Metadata Legend:** A table showing the distribution of concepts across different classes and types.
- Console:** A command-line interface for SPARQL queries.

Concept ID	Color
3694	Purple
39947	Green

Concept Class	Data Sources	Relation Types	Evidence Types
Publication	12 (12)		
TO	7 (7)		
Protein	8 (8)		
Total Concepts 27 (27)			

```
Command console v1.0 Type 'help;' for more information.
ONDEX>sparql_mode
Changing configuration - please wait...
SPARQL interpreter loaded successfully
ONDEX>connect ("http://babvs03.rothamsted.bbsrc.ac.uk:8050/sparql")
ONDEX>construct { ?x ?y "shoot branching"
where { graph ?g { ?x ?y "shoot branching" } }
ONDEX>
ONDEX>
ONDEX>
```



Acknowledgements

- Artem Lysenko
- Andrea Splendiani
- Matthew Pocock
- Chris Rawlings