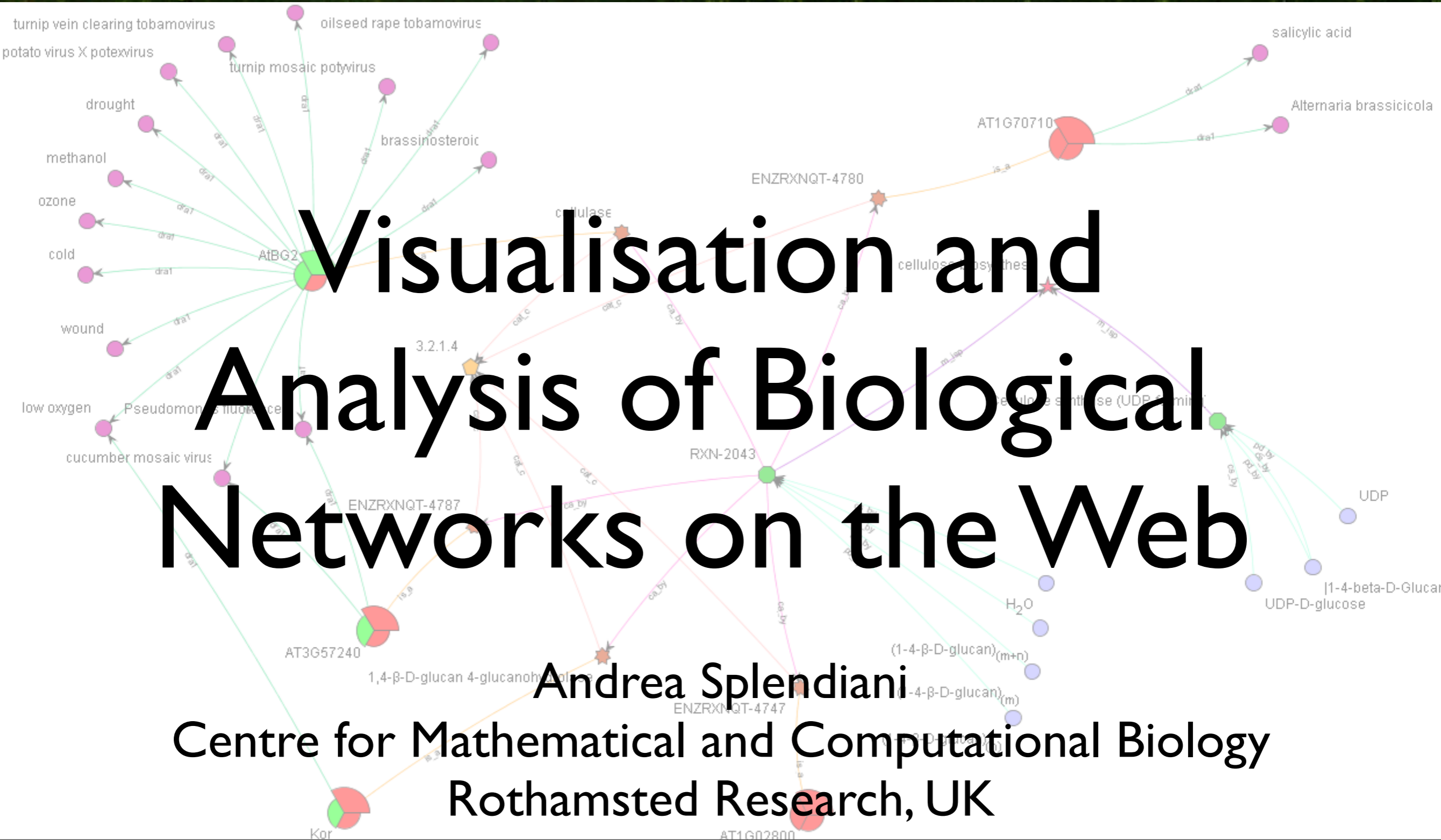




Visualisation and Analysis of Biological Networks on the Web



Andrea Splendiani

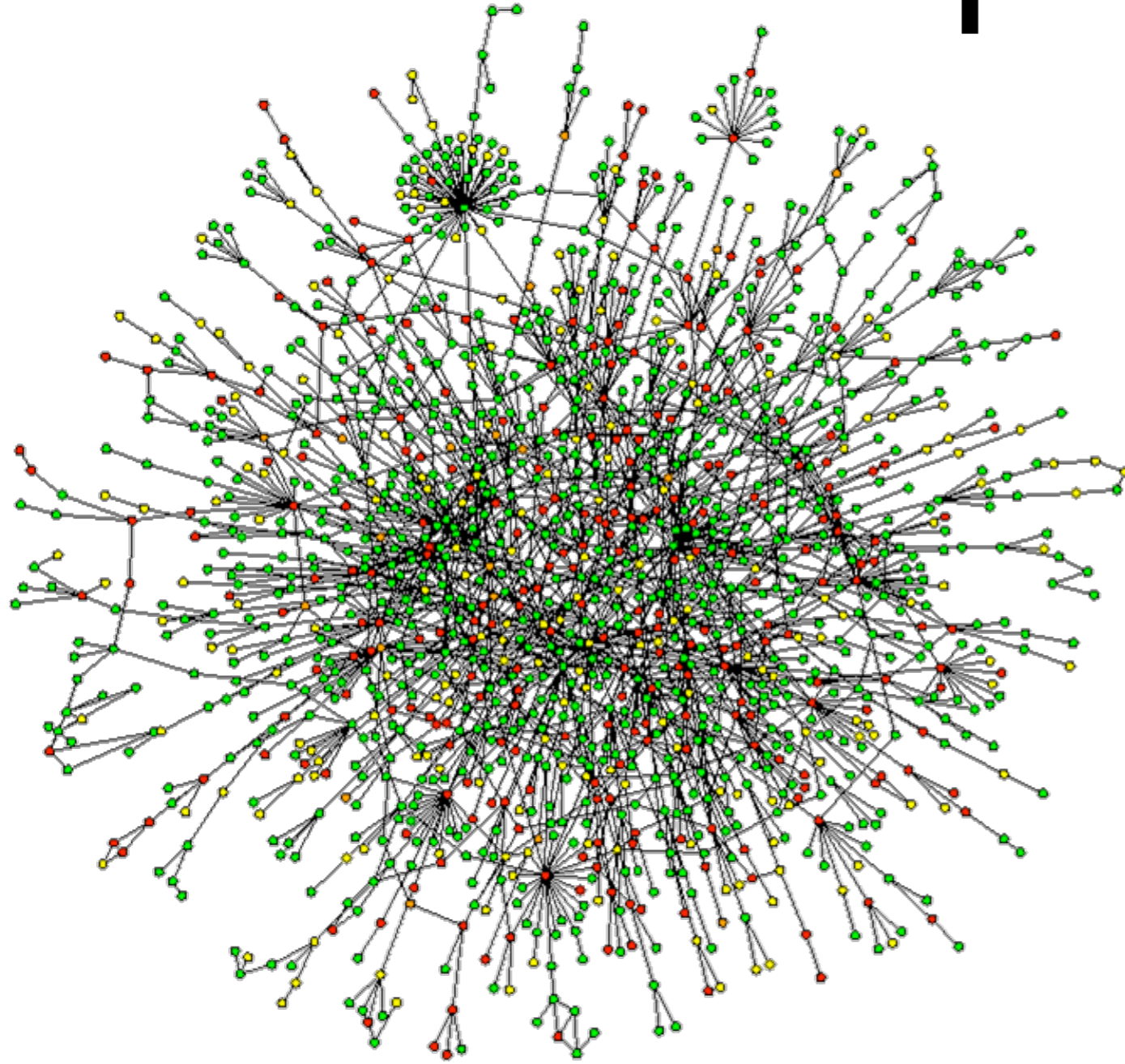
Centre for Mathematical and Computational Biology
Rothamsted Research, UK

The parts



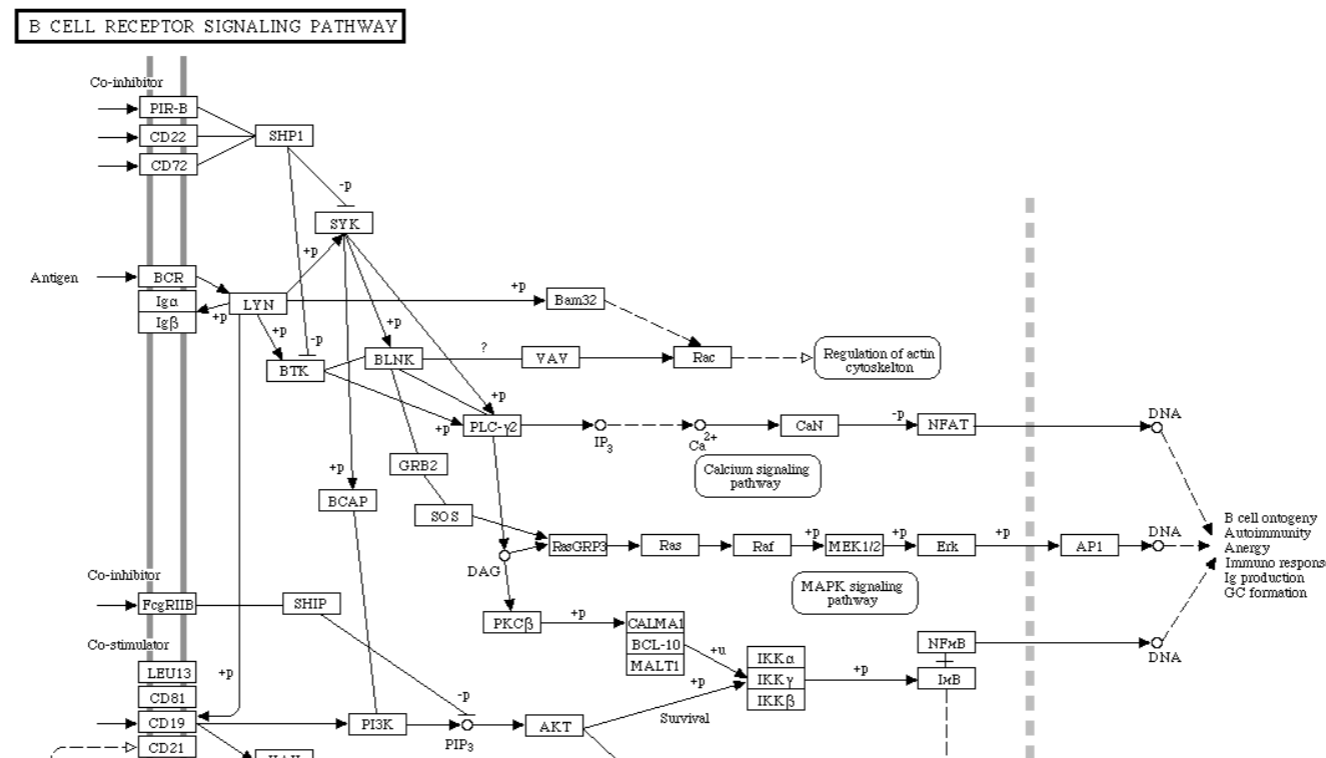
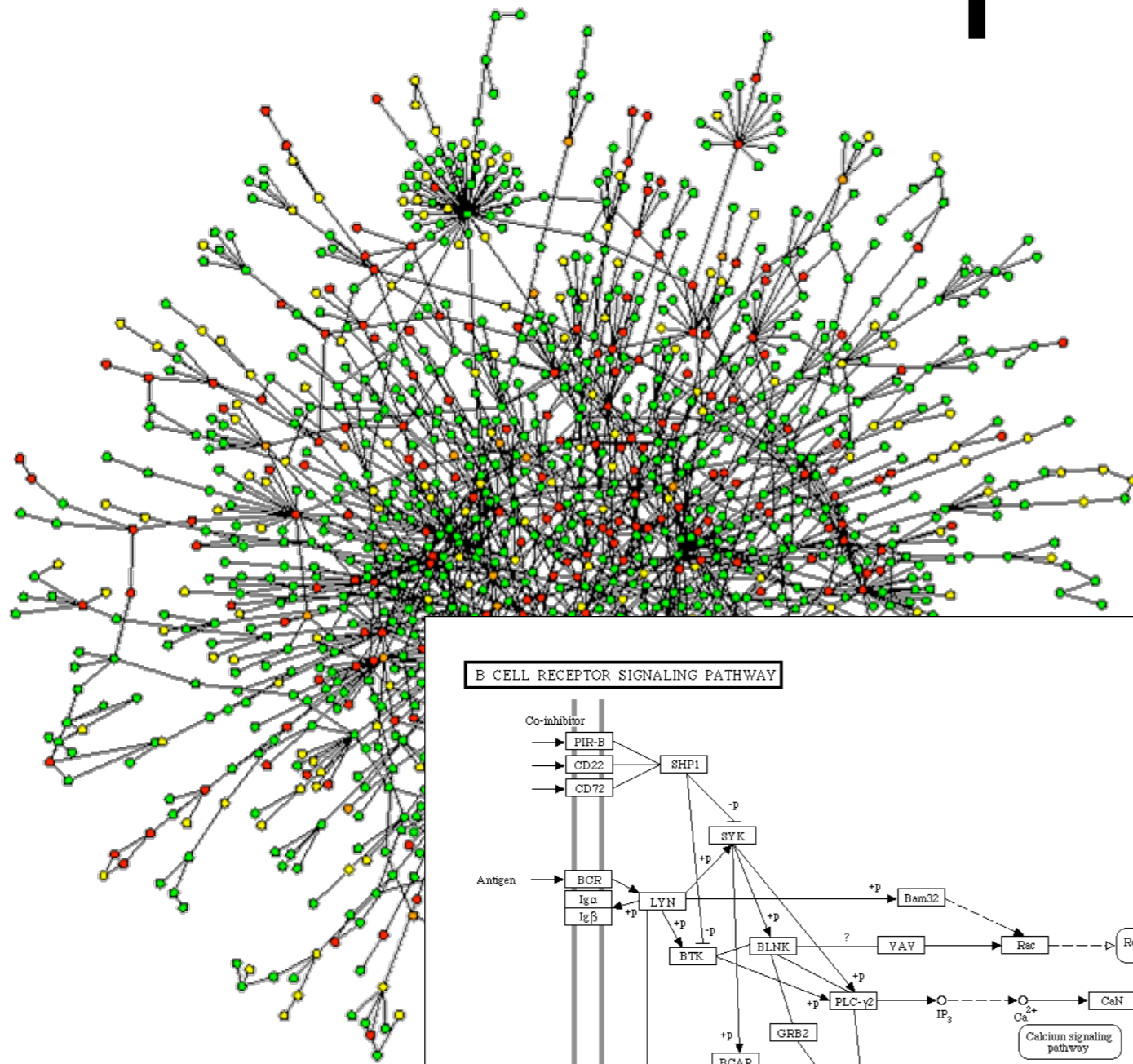
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The parts



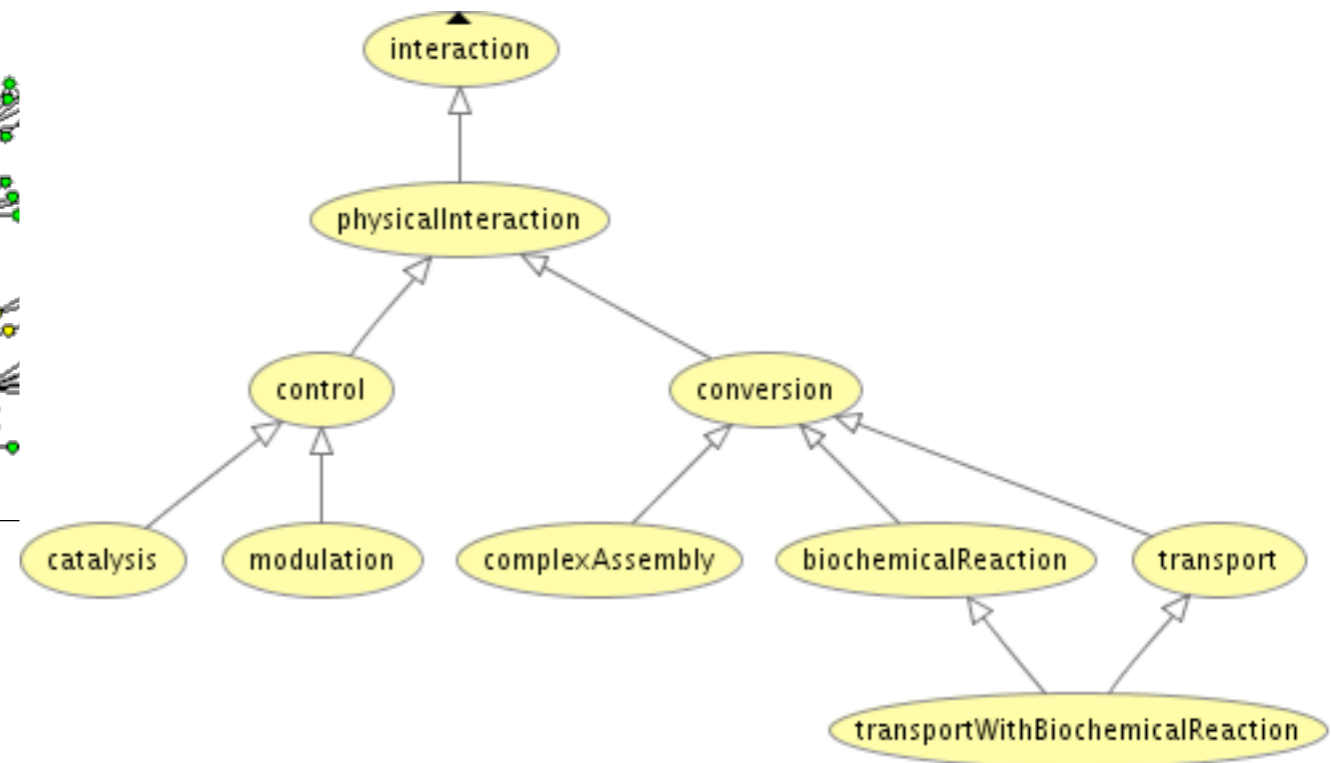
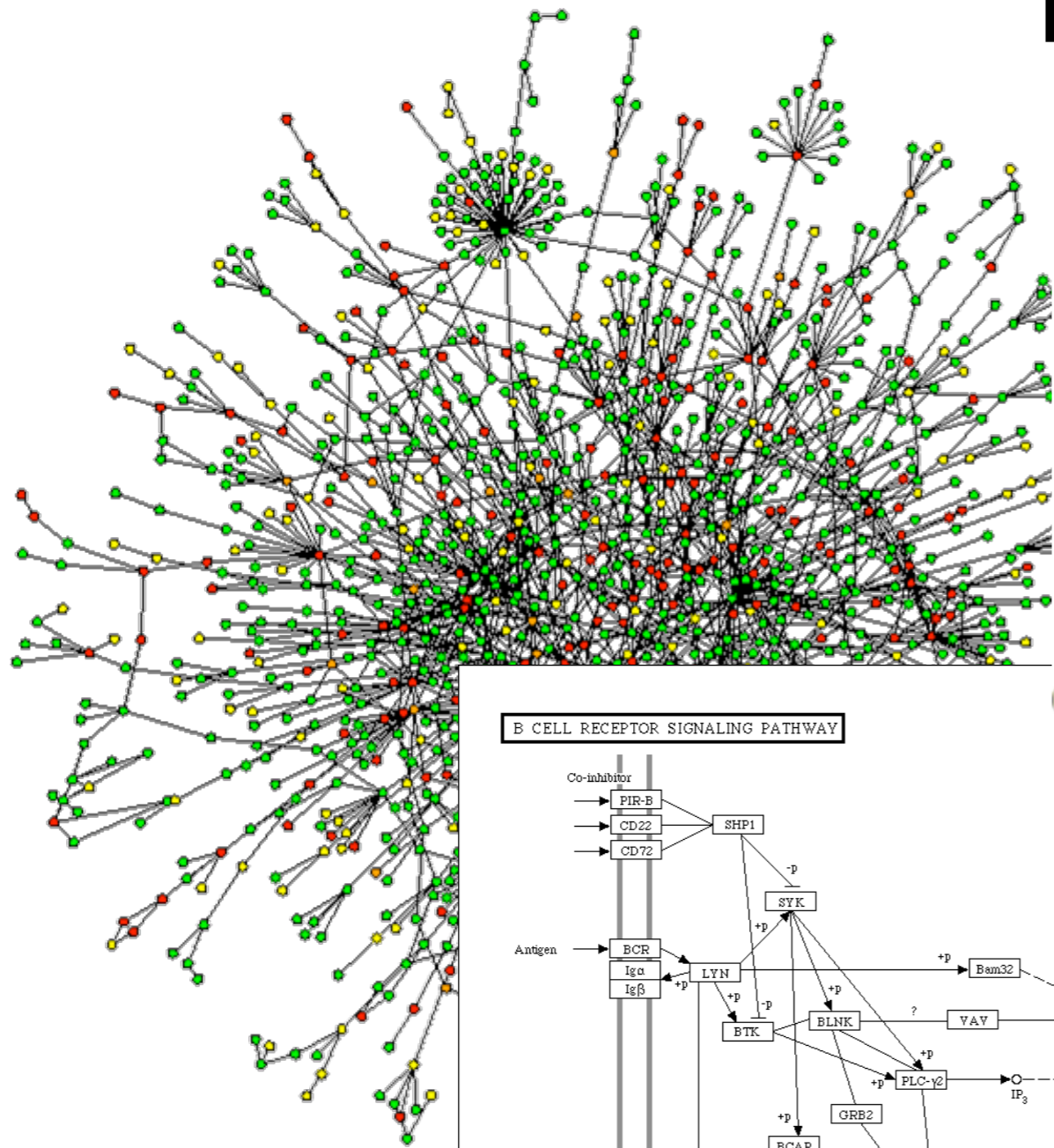
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The parts

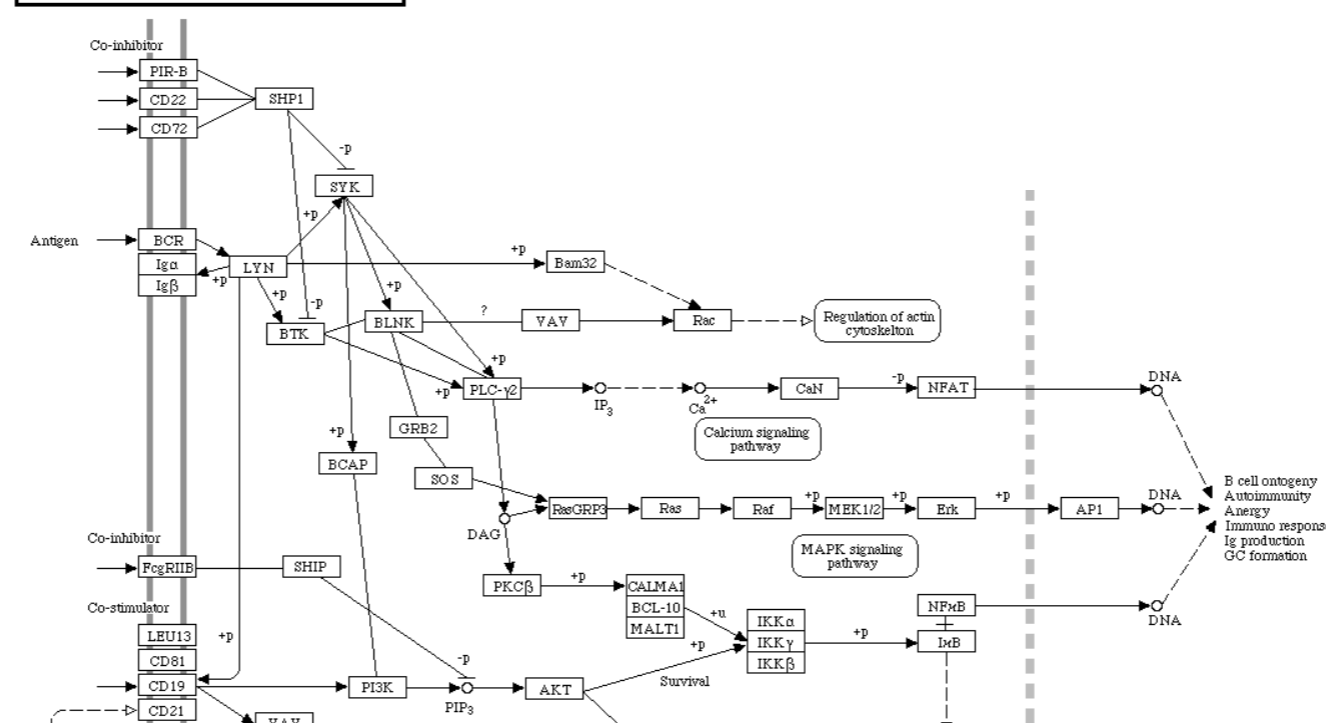


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The parts



B CELL RECEPTOR SIGNALING PATHWAY



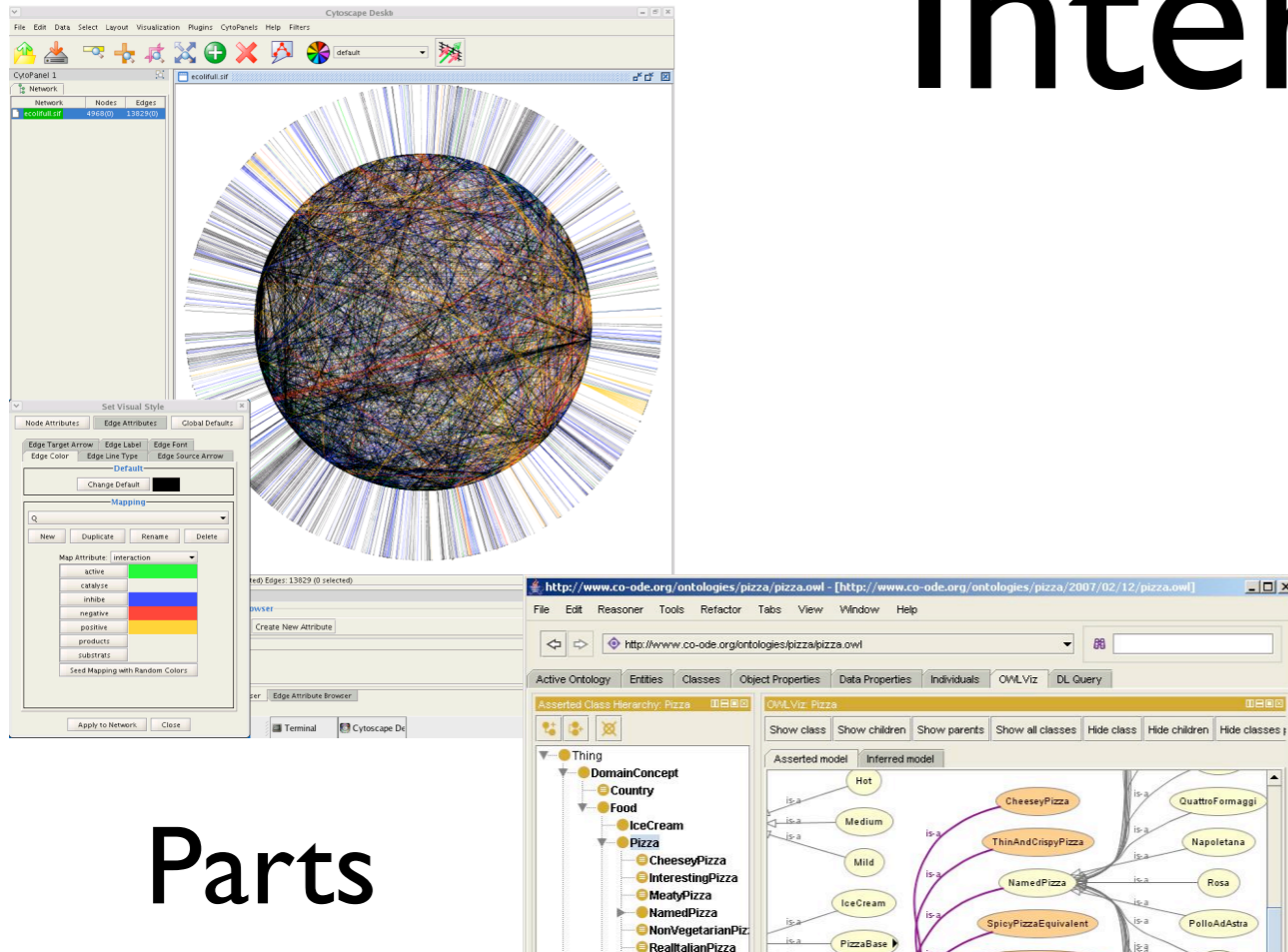
The whole



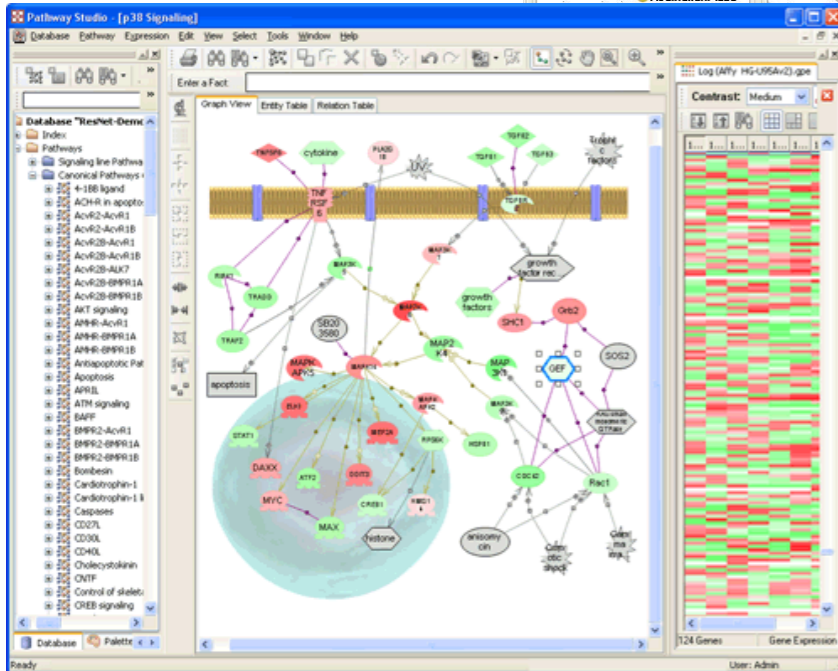
As of March 2009

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Interfaces



Parts



Query

Default Graph URI

Security restrictions of this server do not allow you to retrieve remote RDF data. DBA may wish to grant the user 'SPARQL' the privilege to remove the restriction. In order to do this, please perform the following steps:

1. Go to the Virtuoso Administration Conductor i.e. <http://localhost:8892/conductor>
2. Login as dba user
3. Go to System Admin->User Accounts->Roles
4. Click the link "Edit" for "SPARQL_SPONGE"
5. Select from the list of available user/groups "SPARQL" and click the ">>" button so to add it
6. Click the button "Update"
7. Access again the sparql endpoint in order to be able to retrieve remote data.

Query text

```
SELECT COUNT (distinct ?graph) WHERE {GRAPH ?graph {?s ?p ?o}}
```

Display Results As: Rigorous check of the query

Whole

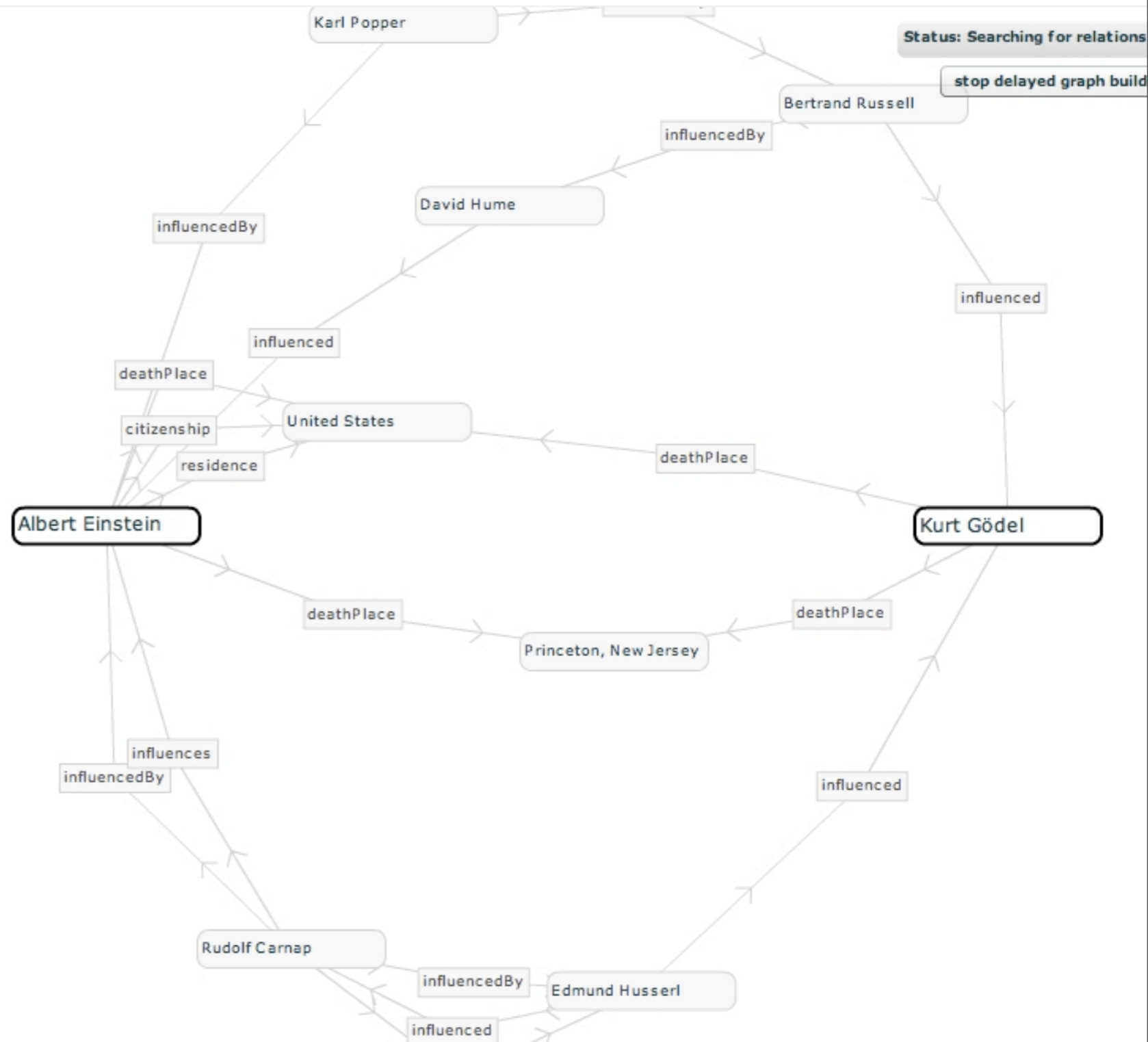
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Interfaces

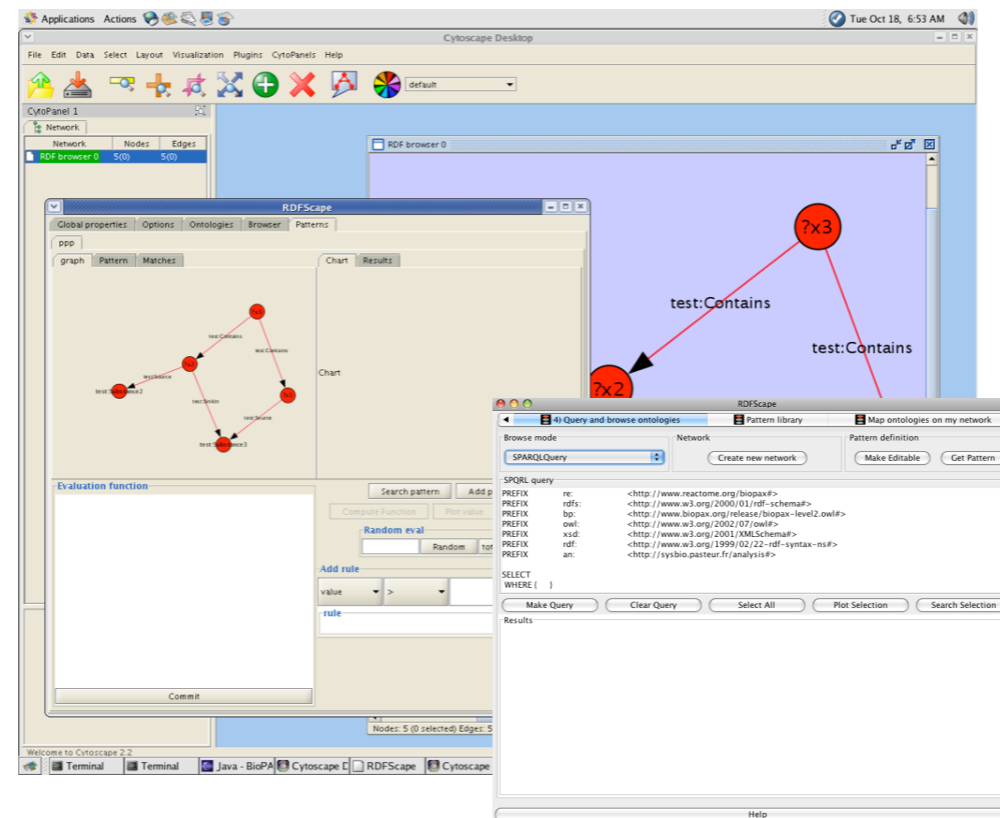
RelFinder interface showing search criteria and filters. The search criteria include "between" and "examples" with input fields for "Albert Einstein" and "Kurt Gödel". The filter section includes "Filter by:" with options for "length", "class", "link", and "conne...". A table displays the number of objects for each filter.

number of objects	num	vi
1	4/4	
2	8/8	

Source:
<http://relfinder.dbpedia.org/>



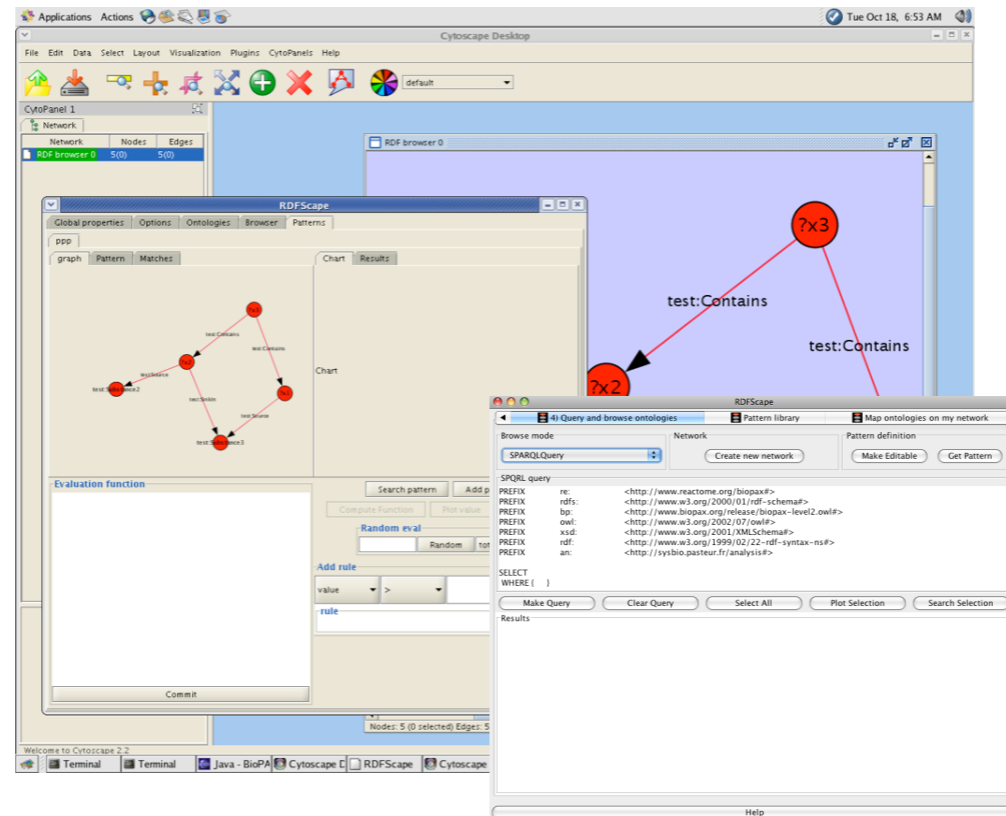
RDFScape



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RDFScape = Interface

Using Cytoscape
for interaction
on the Semantic
Web



Using the
Semantic Web
for the analysis
of networks in
Cytoscape

RDFScape = Interface

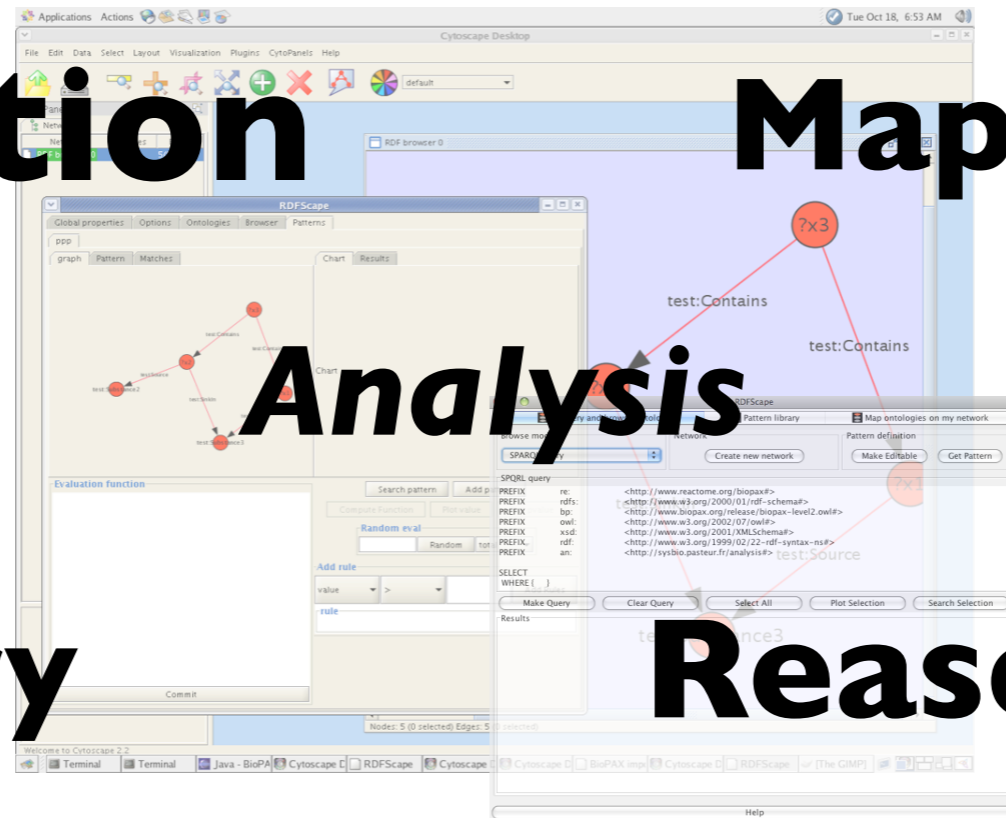
Inspection

Mapping

Analysis

Query

Reasoning



RDFScape = Interface

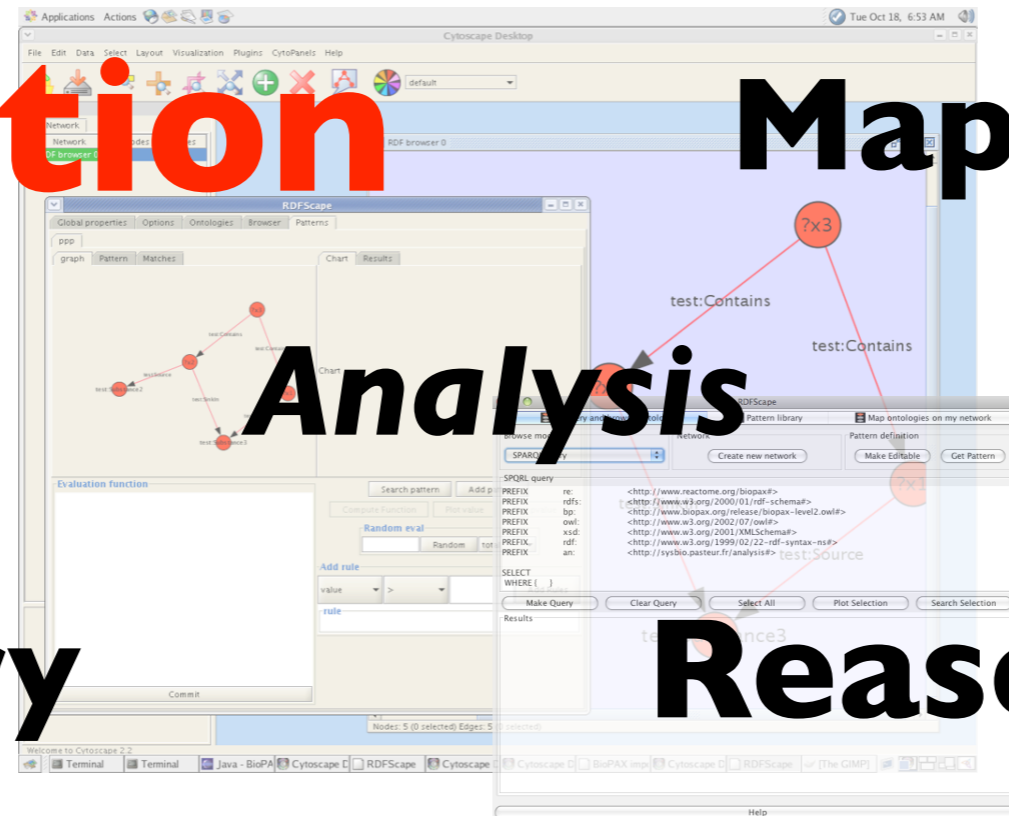
Inspection

Mapping

Analysis

Query

Reasoning



Inspection

The screenshot displays the Cytoscape Desktop interface. The main window, titled "Cytoscape Desktop (New Session)", shows a network diagram with two red circular nodes. The top node is labeled "demo:unificationXref46" and the bottom node is labeled "phosphoglucose isomerase". A blue arrow points from the bottom node to the top node, with the label "biopax2:XREF" positioned between them. To the left of the main window is the "Control Panel" with tabs for "VizMapper™", "Editor", and "Filters". The "VizMapper™" tab is active, showing "Current Visual Style" set to "rdfscape", "Defaults" with a diagram of a box and an arrow, and a "Visual Mapping Browser" with various mapping options. Below the main window is the "Data Panel" with a table structure:

ID	LABEL	URI
----	-------	-----

At the bottom of the interface, there are three tabs: "Node Attribute Browser", "Edge Attribute Browser" (which is selected), and "Network Attribute Browser". The status bar at the very bottom contains the text: "Welcome to Cytoscape 2.7.0 Right-click + drag to ZOOM Middle-click + drag to PAN".

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Inspection

The screenshot displays the Cytoscape Desktop interface. The main window shows a network diagram with two red circular nodes. The top node is labeled "demo:unificationXref46" and the bottom node is labeled "phosphoglucose isomerase". A blue arrow labeled "biopax2:XREF" points from the bottom node to the top node. A context menu is open over the bottom node, showing options: "Visual Mapping Bypass", "Nested Network", "Use Web Services", "LinkOut", and "Extend". A tooltip is visible over the "LinkOut" option, displaying the URL: <http://www.biopax.org/examples/simple-demo-pathway#protein45>. The interface includes a Control Panel on the left with sections for "VizMapper™ Editor", "Current Visual Style" (set to "rdfscape"), "Defaults", and "Visual Mapping Browser". The "Visual Mapping Browser" shows a table of mappings for edges and nodes. The "Data Panel" at the bottom right contains a table with columns for ID, LABEL, and URI. The status bar at the bottom provides instructions: "Welcome to Cytoscape 2.7.0", "Right-click + drag to ZOOM", and "Middle-click + drag to PAN".

Edge Visual Ma...	Node Visual Ma...
Edge Color	Node Color
Edge Label	Node Label
Mapping Type	Node Line Style
http://www....	Node Shape
rdf:type	Unused Properties
http://www....	Edge Font Face
biopax2:XREF	Edge Font Size
	Edge Label Color
	Edge Label Opacity
	Edge Label Width
	Edge Line Style

ID	LABEL	URI
----	-------	-----

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Inspection

The screenshot displays the Cytoscape Desktop interface. The main window shows a network diagram with two red circular nodes. The top node is labeled "demo:unificationXref46" and the bottom node is labeled "phosphoglucose isomerase". A blue directed edge labeled "biopax2:XREF" connects the bottom node to the top node. A context menu is open over the bottom node, showing options: "Me (object)", "Me (subject)", "Extend", "LinkOut", "Use Web Services", "Nested Network", and "Visual Mapping Bypass". A tooltip is visible over the "Extend" option, displaying the URL: <http://www.biopax.org/examples/simple-demo-pathway#protein45>. The left sidebar contains the "Control Panel" with sections for "VizMapper™", "Current Visual Style" (set to "rdfscape"), "Defaults", and "Visual Mapping Browser". The "Visual Mapping Browser" shows a table of mappings for edges and nodes. The "Data Panel" at the bottom is empty, with columns for "ID", "LABEL", and "URI".

Category	Property	Value
Edge Visual Ma...	Edge Color	COLOR
	Edge Label	LABEL
	Mapping Type	Passthrough Mapping
Edge Label	http://www....	rdf:type
	http://www....	biopax2:XREF
Node Visual Ma...	Node Color	COLOR
	Node Label	biopax2:NAME
	Node Line Style	TYPE
	Node Shape	TYPE
Unused Properties	Edge Font Face	Double-Click to cre...
	Edge Font Size	Double-Click to cre...
	Edge Label Color	Double-Click to cre...
	Edge Label Opacity	Double-Click to cre...
	Edge Label Width	Double-Click to cre...
	Edge Line Style	Double-Click to cre...
	Edge Line Width	Double-Click to cre...
	Edge Opacity	Double-Click to cre...

Welcome to Cytoscape 2.7.0 Right-click + drag to ZOOM Middle-click + drag to PAN

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Inspection

The screenshot displays the Cytoscape Desktop interface (New Session) with a network diagram. The diagram features two red circular nodes: 'demo:unificationXref46' at the top and 'phosphoglucose isomerase' at the bottom. A blue arrow labeled 'biopax2:XREF' points from the bottom node to the top node. A context menu is open over the 'phosphoglucose isomerase' node, showing options: 'Extend', 'biopax2:XREF', 'biopax2:COMMENT', 'biopax2:NAME', 'biopax2:SHORT-NAME', 'biopax2:SEQUENCE', 'biopax2:ORGANISM', 'biopax2:AVAILABILITY', 'rdf:type', 'biopax2:DATA-SOURCE', and 'biopax2:SYNONYMS'. A secondary menu is open over the 'Extend' option, listing: 'Visual Mapping Bypass', 'Nested Network', 'Use Web Services', and 'LinkOut'. The 'LinkOut' option is highlighted, and a tooltip shows the URL: <http://www.biopax.org/examples/simple-demo-pathway#protein45>. The interface includes a Control Panel on the left with 'VizMapper™' selected, a Visual Mapping Browser, and a Data Panel at the bottom. The status bar at the bottom indicates 'Welcome to Cytoscape 2.7.0' and provides navigation instructions: 'Right-click + drag to ZOOM' and 'Middle-click + drag to PAN'.

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BioHackathon3 Symposium

Inspection

The screenshot displays the Cytoscape Desktop interface with a network graph. The graph consists of two red circular nodes: 'demo:unificationXref46' at the top and 'phosphoglucose isomerase' at the bottom. A blue arrow labeled 'biopax2:XREF' points from the bottom node to the top node. A context menu is open over the 'phosphoglucose isomerase' node, showing options such as 'Extend', 'biopax2:XREF', 'biopax2:COMMENT', 'biopax2:NAME', 'biopax2:SHORT-NAME', 'biopax2:SEQUENCE', 'biopax2:ORGANISM', 'biopax2:AVAILABILITY', 'rdf:type', 'biopax2:DATA-SOURCE', and 'biopax2:SYNONYMS'. The 'rdf:type' option is highlighted, and a tooltip shows 'Me rdf:type biopax2:protein'. The interface includes a Control Panel on the left with 'VizMapper™' selected, a Data Panel at the bottom, and a footer with navigation instructions.

Control Panel

VizMapper™ Editor Filters

Current Visual Style: rdfscape

Defaults

Visual Mapping Browser

Edge Visual Ma...
Edge Color: COLOR
Edge Label: LABEL
Mapping Type: Passthrough Mapping
http://www.... rdf:type
http://www.... biopax2:XREF

Node Visual Ma...
Node Color: COLOR
Node Label: biopax2:NAME
Node Line Style: TYPE
Node Shape: TYPE

Unused Properties

Edge Font Face: Double-Click to cre...
Edge Font Size: Double-Click to cre...
Edge Label Color: Double-Click to cre...
Edge Label Opacity: Double-Click to cre...
Edge Label Width: Double-Click to cre...
Edge Line Style: Double-Click to cre...

Search: []

RDFScape ontology browser # 2

demo:unificationXref46

biopax2:XREF

phosphoglucose isomerase

<http://www.biopax.org/examples/simple-demo-pathway#protein45>

Visual Mapping Bypass
Nested Network
Use Web Services

LinkOut

Me (object) ▶ Extend
Me (subject) ▶ biopax2:XREF
biopax2:COMMENT
biopax2:NAME
biopax2:SHORT-NAME
biopax2:SEQUENCE
biopax2:ORGANISM
biopax2:AVAILABILITY
rdf:type ▶ Me rdf:type biopax2:protein
biopax2:DATA-SOURCE
biopax2:SYNONYMS

Data Panel

ID

Node Attribute Browser Edge Attribute Browser Network Attribute Browser

Welcome to Cytoscape 2.7.0 Right-click + drag to ZOOM Middle-click + drag to PAN

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Inspection

The screenshot displays the Cytoscape Desktop interface with a new session. The main window shows a graph visualization with three nodes: a red node labeled 'demo:unificationXref46', a red node labeled 'phosphoglucose isomerase', and a blue node labeled 'biopax2:protein'. The edges are labeled 'biopax2:XREF' (connecting the top two nodes) and 'rdf:type' (connecting the middle and bottom nodes).

The left sidebar contains the Control Panel with the following sections:

- VizMapper™ Editor**: Current Visual Style is 'rdfscape'.
- Defaults**: Shows a default node and edge representation.
- Visual Mapping Browser**:
 - Edge Visual Ma...**:
 - Edge Color: COLOR
 - Edge Label: LABEL
 - Mapping Type: Passthrough Mapping
 - http://www....: rdf.type
 - http://www....: biopax2:XREF
 - Node Visual Ma...**:
 - Node Color: COLOR
 - Node Label: biopax2:NAME
 - Node Line Style: TYPE
 - Node Shape: TYPE
 - Unused Properties**:
 - Edge Font Face: Double-Click to cre...
 - Edge Font Size: Double-Click to cre...
 - Edge Label Color: Double-Click to cre...
 - Edge Label Opacity: Double-Click to cre...
 - Edge Label Width: Double-Click to cre...
 - Edge Line Style: Double-Click to cre...

The bottom right of the interface features the Data Panel with a table structure:

ID	LABEL	URI
----	-------	-----

Navigation buttons at the bottom include 'Node Attribute Browser', 'Edge Attribute Browser', and 'Network Attribute Browser'. The status bar at the very bottom provides instructions: 'Welcome to Cytoscape 2.7.0', 'Right-click + drag to ZOOM', and 'Middle-click + drag to PAN'.

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RDFScape = Interface

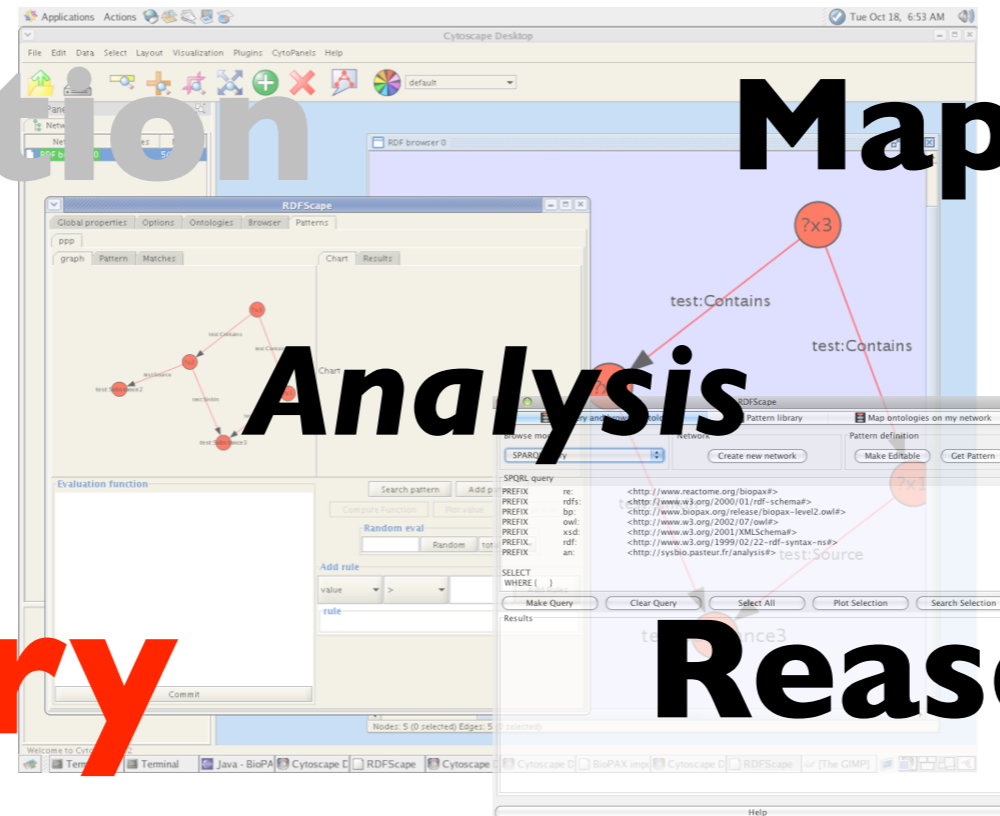
Inspection

Mapping

Analysis

Query

Reasoning



Query

The screenshot displays the Cytoscape Desktop interface. The main window shows a network visualization with three nodes: a yellow node labeled 'biopax2:protein', a red node labeled 'demo:bioSource33', and a red node labeled 'demo:protein32'. Edges connect 'demo:protein32' to 'biopax2:protein' (labeled 'rdf:type') and 'demo:protein32' to 'demo:bioSource33' (labeled 'biopax2:ORGANISM').

The Control Panel on the left shows a table with the following data:

Network	Edges	Nodes
RDFScape ontology browser3(0)		9(0)

The Data Panel at the bottom shows a table with the following data:

ID	DATATYPE	LABEL	URI
http://www.biopax.org/release/biopax-level-3		biopax2:protein	http://...

At the bottom of the interface, there are instructions: 'Welcome to Cytoscape 2.7.0', 'Right-click + drag to ZOOM', and 'Middle-click + drag to PAN'. There are also buttons for 'Node Attribute Browser', 'Edge Attribute Browser', and 'Network Attribute Browser'.

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Query

The screenshot displays the Cytoscape Desktop interface (New Session) with a network visualization and an RDFScope ontology browser window. The network shows three nodes: `biopax2:protein` (blue), `demo:bioSource33` (red), and `demo:protein32` (red). Edges connect `demo:protein32` to `biopax2:protein` (labeled `rdf:type`) and `demo:protein32` to `demo:bioSource33` (labeled `biopax2:ORGANISM`). A context menu is open over the `demo:protein32` node, listing options: `http://www.biopax.org/examples/simple-demo-pathway#protein32`, `Visual Mapping Bypass`, `Nested Network`, `Use Web Services`, `LinkOut`, `Make variable` (highlighted), and `Extend`. The Data Panel at the bottom shows a table with columns: ID, DATATYPE, LABEL, and URI. The interface also includes a Control Panel with a Network tab and a VizMapper™ window.

Control Panel

Network Edges Nodes

RDFScope ontology browser2(0) 3(1)

RDFScope ontology browser # 1

biopax2:protein

demo:bioSource33

demo:protein32

rdf:type

biopax2:ORGANISM

<http://www.biopax.org/examples/simple-demo-pathway#protein32>

Visual Mapping Bypass

Nested Network

Use Web Services

LinkOut

Make variable

Extend

Data Panel

ID	DATATYPE	LABEL	URI
----	----------	-------	-----

Node Attribute Browser Edge Attribute Browser Network Attribute Browser

Welcome to Cytoscape 2.7.0 Right-click + drag to ZOOM Middle-click + drag to PAN

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BioHackathon3 Symposium

Query

The screenshot displays the Cytoscape Desktop interface. The main window shows a network visualization with three nodes: a blue node labeled 'biopax2:protein', a red node labeled 'demo:bioSource33', and a grey node with a question mark. Edges connect the grey node to both the blue and red nodes, labeled 'rdf:type' and 'biopax2:ORGANISM' respectively. A smaller window titled 'RDFScape ontology browser # 1' shows the same network structure. The Control Panel on the left lists the network as 'RDFScape ontology browser2(0)' with 3 nodes and 1 edge. The Data Panel at the bottom shows a table with columns for ID, DATATYPE, LABEL, and URI. The interface also includes a search bar, a user profile for 'Enrica' (came online), and navigation instructions at the bottom: 'Welcome to Cytoscape 2.7.0', 'Right-click + drag to ZOOM', and 'Middle-click + drag to PAN'.

Control Panel

Network	Edges	Nodes
RDFScape ontology browser2(0)		3(1)

RDFScape ontology browser # 1

biopax2:protein

demo:bioSource33

rdf:type

biopax2:ORGANISM

?

biopax2:protein

demo:bioSource

rdf:type

biopax2:ORGANISM

?

Data Panel

ID	DATATYPE	LABEL	URI
----	----------	-------	-----

Node Attribute Browser Edge Attribute Browser Network Attribute Browser

Welcome to Cytoscape 2.7.0 Right-click + drag to ZOOM Middle-click + drag to PAN

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BioHackathon3 Symposium

Query

The screenshot displays the Cytoscape Desktop interface. The main window shows a network visualization with three nodes: a blue node labeled 'biopax2:protein', a red node labeled 'demo:bioSource33', and a grey node with a question mark. Edges connect the grey node to both the blue and red nodes, with labels 'rdf:type' and 'biopax2:ORGANISM' respectively. A context menu is open over the grey node, listing options: 'Visual Mapping Bypass', 'Use Web Services', 'LinkOut', and 'Make variable' (highlighted).

The Control Panel on the left shows a table with the following data:

Network	Edges	Nodes
RDFScape ontology browser2(0)		3(1)

The Data Panel at the bottom shows a table with the following headers:

ID	DATATYPE	LABEL	URI
----	----------	-------	-----

At the bottom of the interface, there are instructions: 'Welcome to Cytoscape 2.7.0', 'Right-click + drag to ZOOM', and 'Middle-click + drag to PAN'. Below these are buttons for 'Node Attribute Browser', 'Edge Attribute Browser', and 'Network Attribute Browser'.

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Query

The screenshot displays the Cytoscape Desktop interface. The main window shows a network visualization with a blue node labeled 'biopax2:protein' and two grey nodes labeled '?'. A green edge labeled 'rdf:type' connects the bottom grey node to the blue node, and a grey edge labeled '?' connects the bottom grey node to the top grey node. A smaller window titled 'RDFScape ontology browser # 1' shows the same network structure. The Control Panel on the left shows a table with columns 'Network', 'Edges', and 'Nodes'. The Data Panel at the bottom shows a table with columns 'ID', 'DATATYPE', 'LABEL', and 'URI'. The bottom status bar includes the text 'Welcome to Cytoscape 2.7.0', 'Right-click + drag to ZOOM', and 'Middle-click + drag to PAN'.

Network	Edges	Nodes
RDFScape ontology browser2(0)		3(1)

ID	DATATYPE	LABEL	URI
----	----------	-------	-----

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Query

Cytoscape Desktop (New Session)

Control Panel

Network | VizMapper™

Network	Edges	Nodes
RDFScape ontology browser2(0)		3(0)

biopax2:protein

rdf:type

?

RDFScape

4) Query and browse ontologies | Pattern library | Map ontologies o

ProteinsAndAttributes

graph | Pattern | Matches

biopax2:protein

rdf:type

?

Search variables | Add variables | Search patterns | Add patterns | Delete pattern

Data Panel

ID	DATA
----	------

Welcome to Cytoscape 2.7.0 | Right-click + drag to ZOOM | Middle-click + drag to PAN

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Query

The image displays a Cytoscape Desktop window with a network visualization and an RDF query interface. The network visualization shows a complex graph of nodes and edges, with nodes labeled with terms like 'glucokinase', 'GLK', 'phosphoglucose isomerase', and 'GPI'. The RDF query interface shows a query pattern with variables and a 'Delete pattern' button.

Control Panel

Network	Edges	Nodes
RDFScape ontology browser	27(0)	23(0)

RDFScape ontology browser # 1

RDFScape

4) Query and browse ontologies | Pattern library | Map ontologies o

ProteinsAndAttributes

graph | Pattern | Matches

biopax2:protein

rdf:type

Search variables | Add variables | Search patterns | Add patterns | Delete pattern

Data Panel

ID	DATA
----	------

Node Attribute Bro

Welcome to Cytoscape 2.7.0 | Right-click + drag to ZOOM | Middle-click + drag to PAN

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RDFScape = Interface

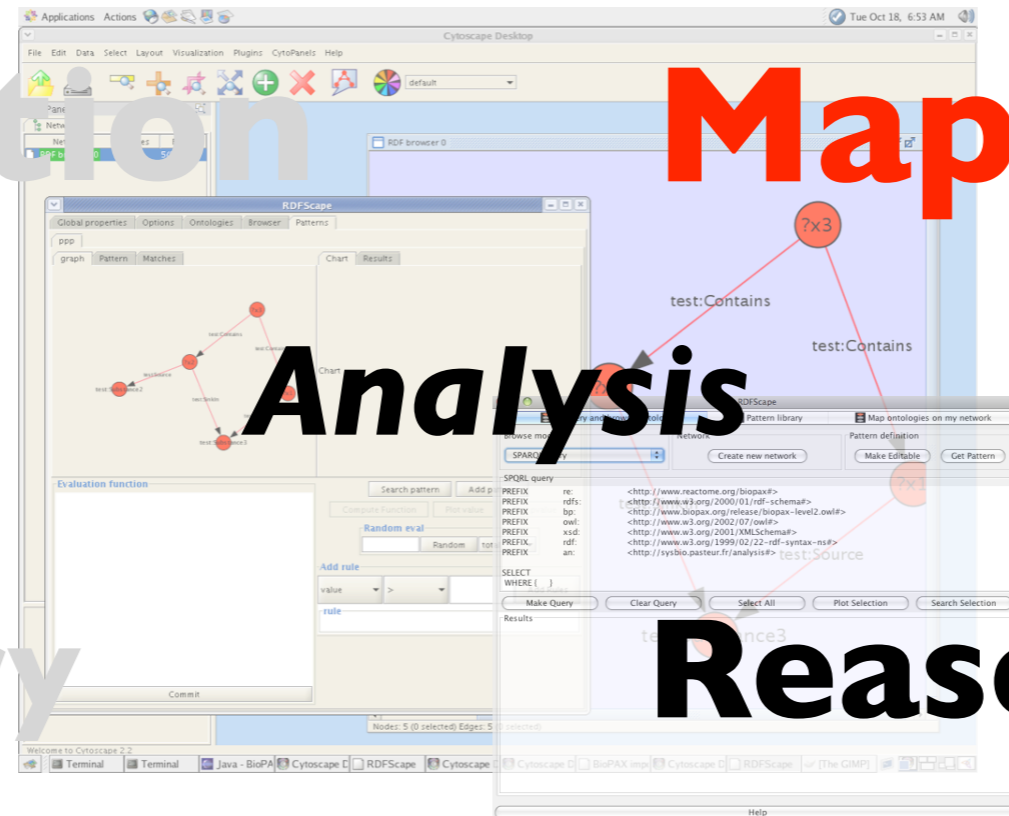
Inspection

Mapping

Analysis

Query

Reasoning



Mapping

The screenshot displays the Cytoscape Desktop interface with a network graph and the RDFScope ontology browser. The graph shows nodes for 'glucokinase', 'phosphoglucose isomerase', 'Escherichia coli', and 'MAZE', connected by edges representing relationships like 'rdf:type' and 'biopax2:XREF'. The RDFScope browser shows a list of namespaces with their prefixes and colors.

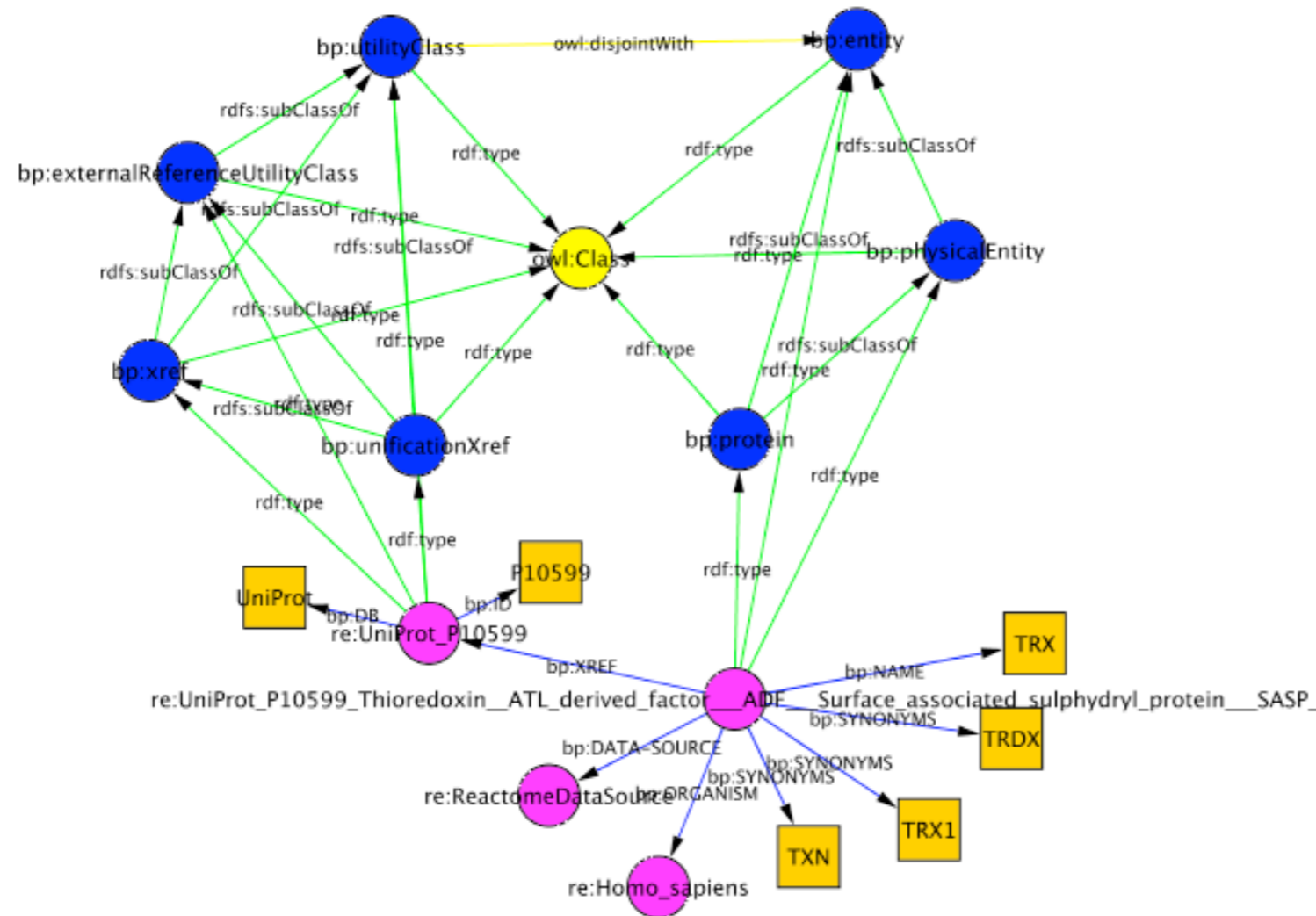
Namespace	Prefix	Color	View
http://www.biopax.org/release/biopax-level3.owl#	biopax3	Red	<input checked="" type="checkbox"/>
http://www.w3.org/2000/01/rdf-schema#	rdfs	Purple	<input checked="" type="checkbox"/>
http://www.w3.org/2003/11/swrl#	ns0	Red	<input type="checkbox"/>
http://protege.stanford.edu/plugins/owl/protege#	ns1	Red	<input type="checkbox"/>
http://www.owl-ontologies.com/2005/08/07/xsp.owl#	ns2	Red	<input type="checkbox"/>
http://www.w3.org/2003/11/swrlb#	ns3	Red	<input type="checkbox"/>
http://www.w3.org/2001/XMLSchema#	xmls	Yellow	<input checked="" type="checkbox"/>
http://www.w3.org/2002/07/owl#	owl	Green	<input checked="" type="checkbox"/>
http://www.w3.org/1999/02/22-rdf-syntax-ns#	rdf	Green	<input checked="" type="checkbox"/>
http://www.biopax.org/examples/simple-demo-pathway#	demo	Red	<input checked="" type="checkbox"/>
http://www.biopax.org/release/biopax-level2.owl#	biopax2	Blue	<input checked="" type="checkbox"/>

The Data Panel at the bottom shows a table with columns: biopax2:COMMENT, DATATYPE, LABEL, URI, biopax2:AVAILABILITY, and biopax2:DB.

biopax2:COMMENT	DATATYPE	LABEL	URI	biopax2:AVAILABILITY	biopax2:DB
This example is meant to provide an illustration...	demo:protein32		http://...	see http://www.amaze...	
This example is meant to provide an illustration...	demo:unificationXref35		http://...		Swiss-Prot/TrEMBL
This example is meant to provide an illustration...	demo:bioSource33		http://...		

- selection/colouring by namespace
- datatype properties as attributes
- URIs represented as multiple nodes

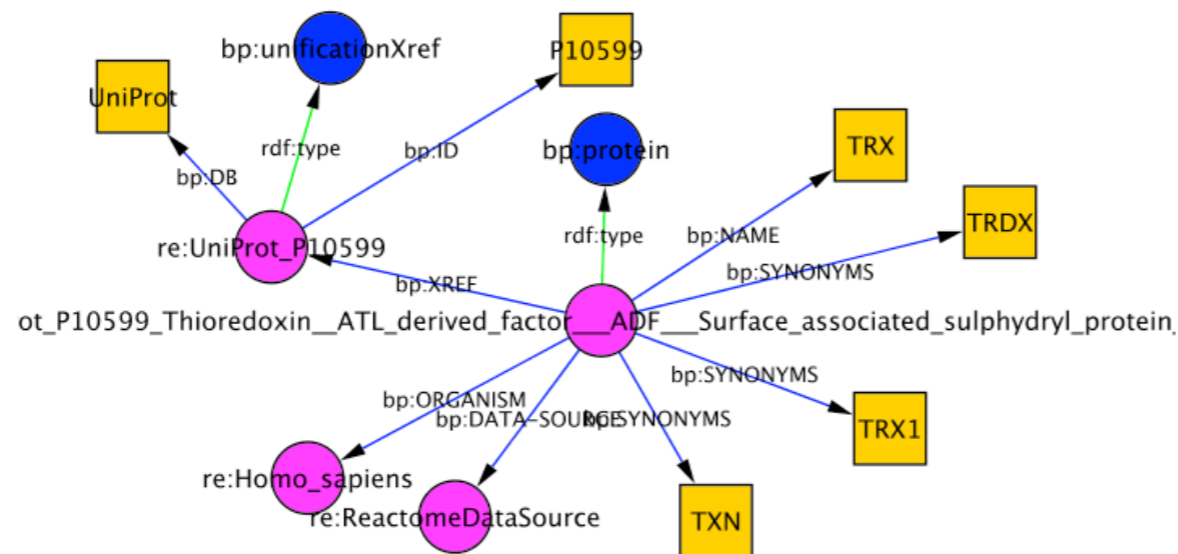
Mapping



- selection/colouring by namespace
- datatype properties as attributes
- URIs represented as multiple nodes

Mapping

- selection/colouring by namespace
- datatype properties as attributes
- URIs represented as multiple nodes



Mapping

The screenshot displays the Cytoscape Desktop interface with a network graph and the RDFScope ontology browser. The graph shows nodes for 'glucokinase', 'phosphoglucose isomerase', 'Escherichia coli', and 'MAZE', connected by edges representing relationships like 'rdf:type' and 'biopax2:XREF'. The RDFScope browser shows a list of namespaces with their prefixes and colors.

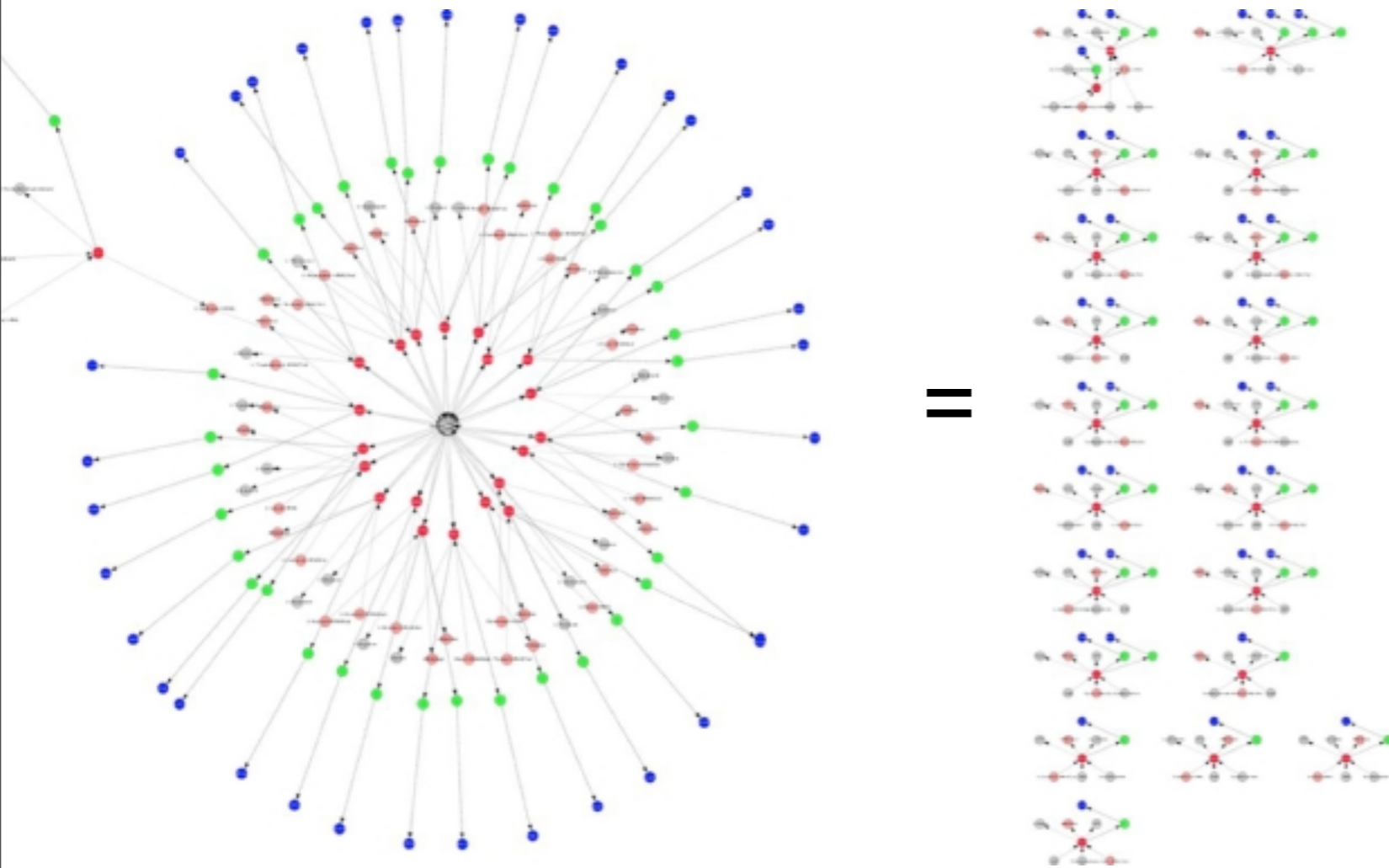
Namespace	Prefix	Color	View
http://www.biopax.org/release/biopax-level3.owl#	biopax3	Red	<input checked="" type="checkbox"/>
http://www.w3.org/2000/01/rdf-schema#	rdfs	Pink	<input checked="" type="checkbox"/>
http://www.w3.org/2003/11/swrl#	ns0	Red	<input type="checkbox"/>
http://protege.stanford.edu/plugins/owl/protege#	ns1	Red	<input type="checkbox"/>
http://www.owl-ontologies.com/2005/08/07/xsp.owl#	ns2	Red	<input type="checkbox"/>
http://www.w3.org/2003/11/swrlb#	ns3	Red	<input type="checkbox"/>
http://www.w3.org/2001/XMLSchema#	xmls	Yellow	<input checked="" type="checkbox"/>
http://www.w3.org/2002/07/owl#	owl	Yellow	<input checked="" type="checkbox"/>
http://www.w3.org/1999/02/22-rdf-syntax-ns#	rdf	Green	<input checked="" type="checkbox"/>
http://www.biopax.org/examples/simple-demo-pathway#	demo	Red	<input checked="" type="checkbox"/>
http://www.biopax.org/release/biopax-level2.owl#	biopax2	Blue	<input checked="" type="checkbox"/>

The Data Panel at the bottom shows a table with columns: biopax2:COMMENT, DATATYPE, LABEL, URI, biopax2:AVAILABILITY, and biopax2:DB.

biopax2:COMMENT	DATATYPE	LABEL	URI	biopax2:AVAILABILITY	biopax2:DB
This example is meant to provide an illustration...	demo:protein32		http://...	see http://www.amaze...	
This example is meant to provide an illustration...	demo:unificationXref35		http://...		Swiss-Prot/TrEMBL
This example is meant to provide an illustration...	demo:bioSource33		http://...		

- selection/colouring by namespace
- datatype properties as attributes
- URIs represented as multiple nodes

Mapping



ATP, H₂O...

- selection/colouring by namespace
- datatype properties as attributes
- **URIs** represented as multiple nodes

RDFScape = Interface

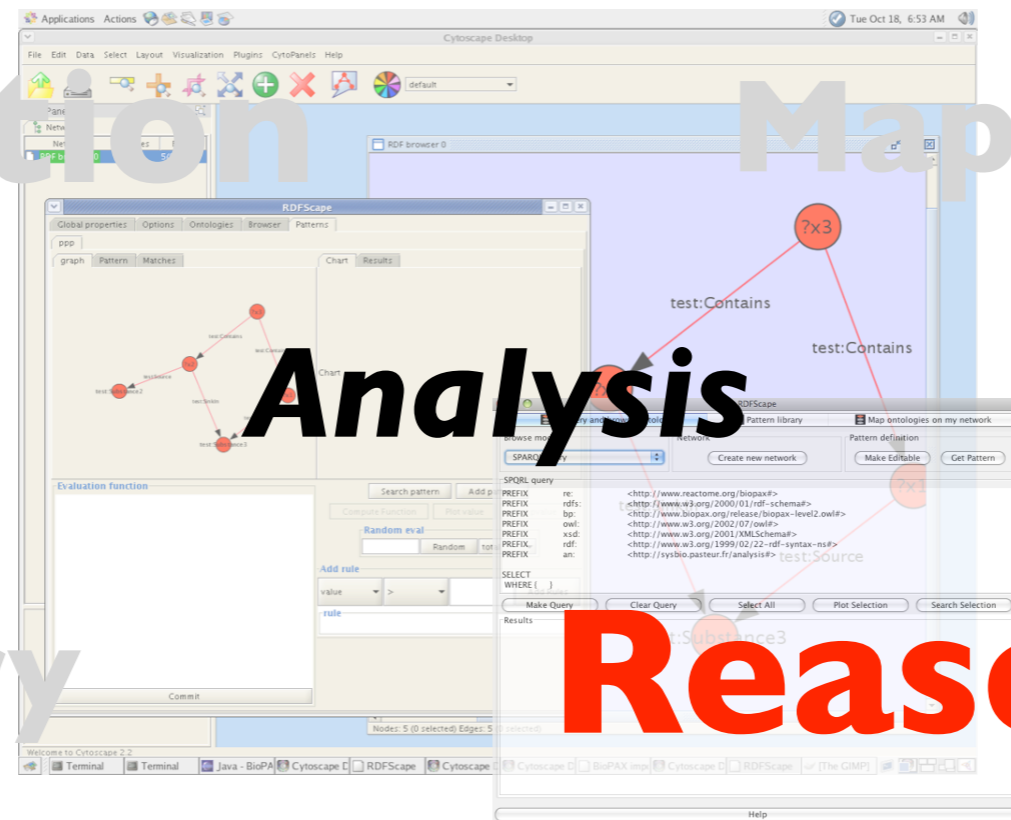
Inspection

Mapping

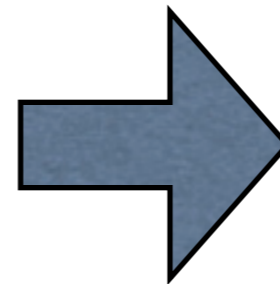
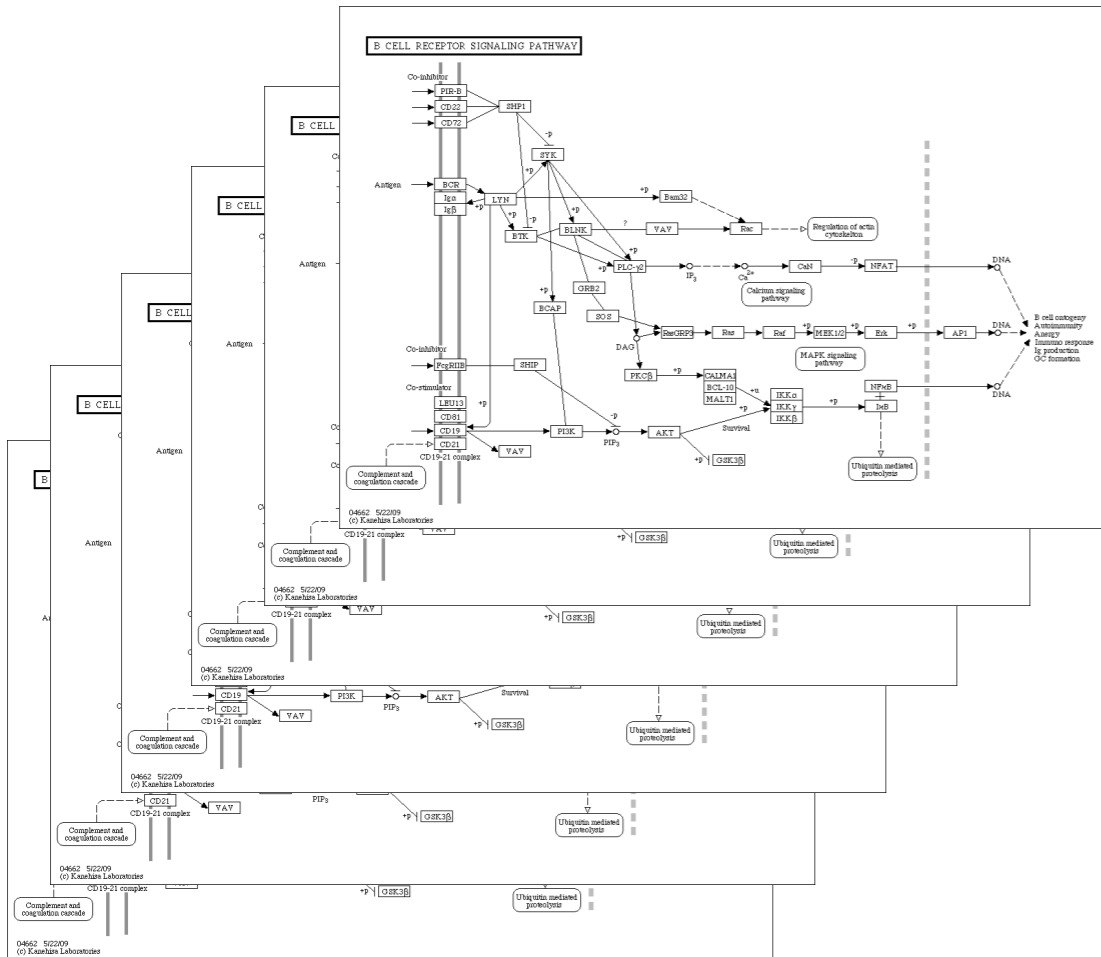
Analysis

Query

Reasoning



Reasoning

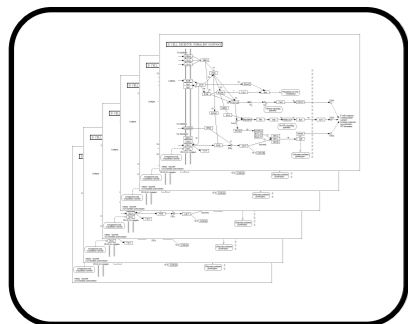


?x6

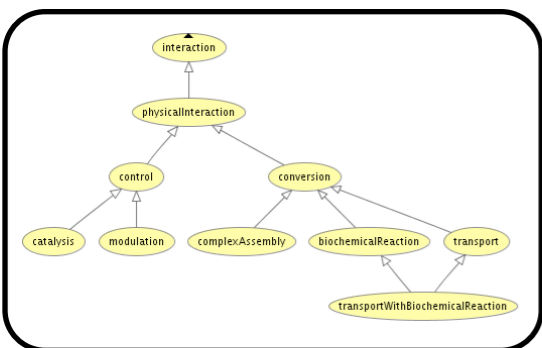
new.interacts

?x7

Reasoning



A collection of pathways:
biological facts



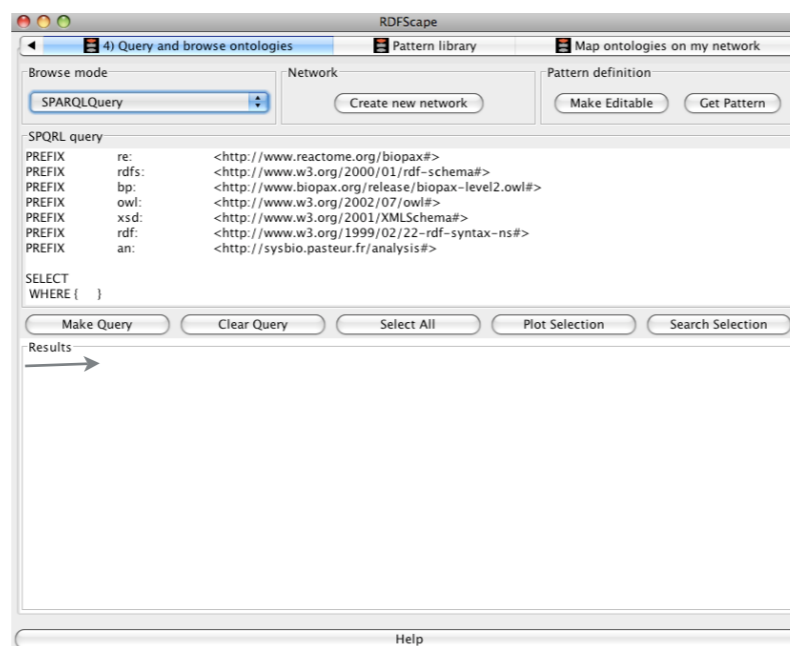
An ontology: a meaning
for facts (interpretation)

```
[Skip-Context1:  
(?i an:directp ?p) <- (?i bp:PARTICIPANT ?p)  
(?p rdf:type bp:entity)]
```

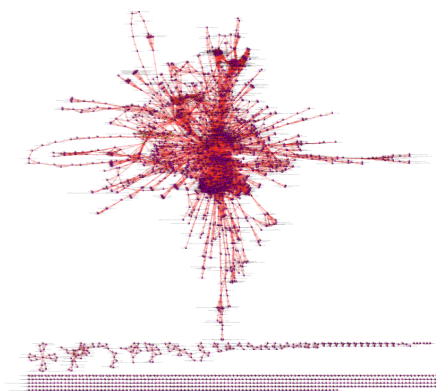
```
[Skip-Context2:  
(?i an:directp ?p) <- (?i bp:PARTICIPANTS ?pep)  
(?pep bp:PHYSICALENTITY ?p)  
(?p rdf:type bp:entity)]
```

```
[Interacts:  
(?x an:interacts ?y) <- (?z rdf:type bp:interaction)  
(?z and:directp ?x) (?z an:directp ?y)]
```

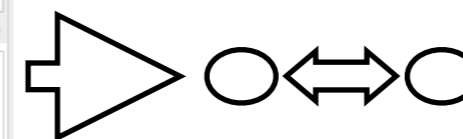
inference rules:
more meaning...



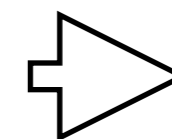
“Semantic-enabled”
Interface (RDFScape)



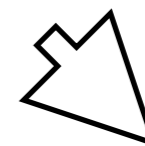
Visualization



Abstraction of pathways
as interactions

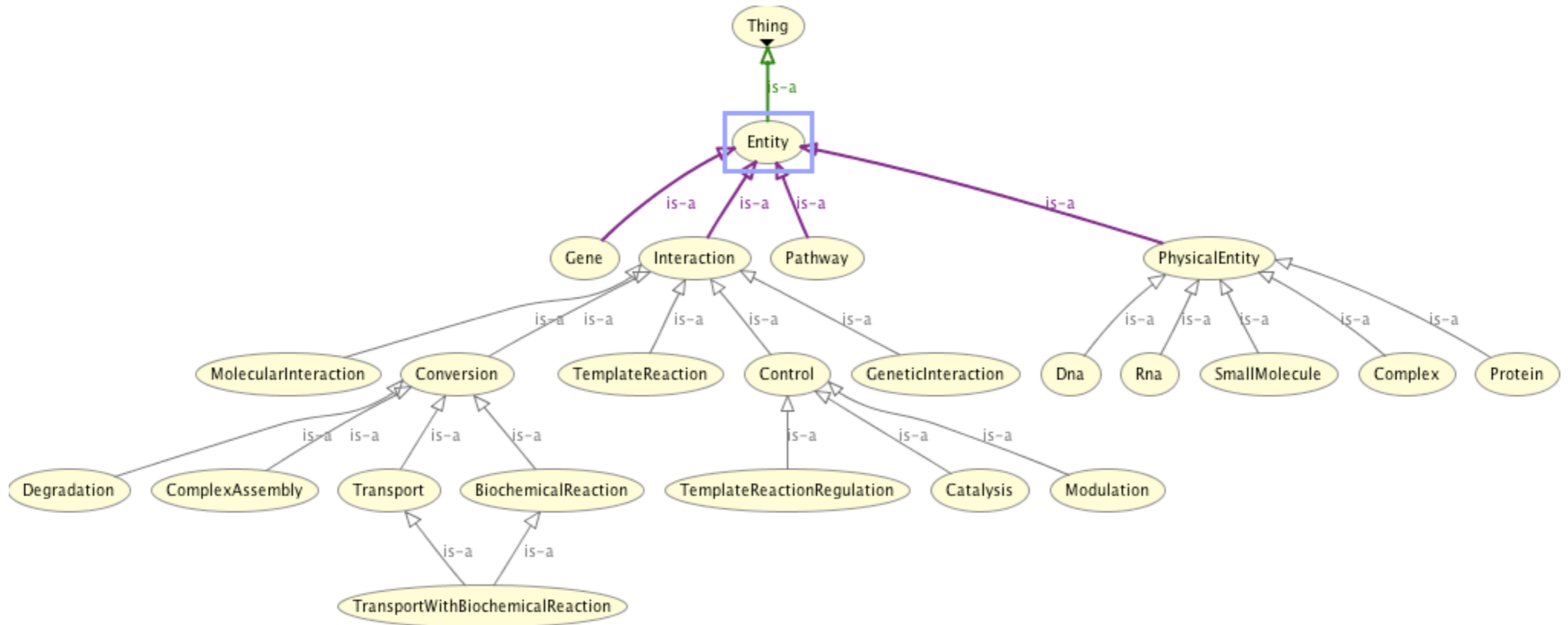


Analysis

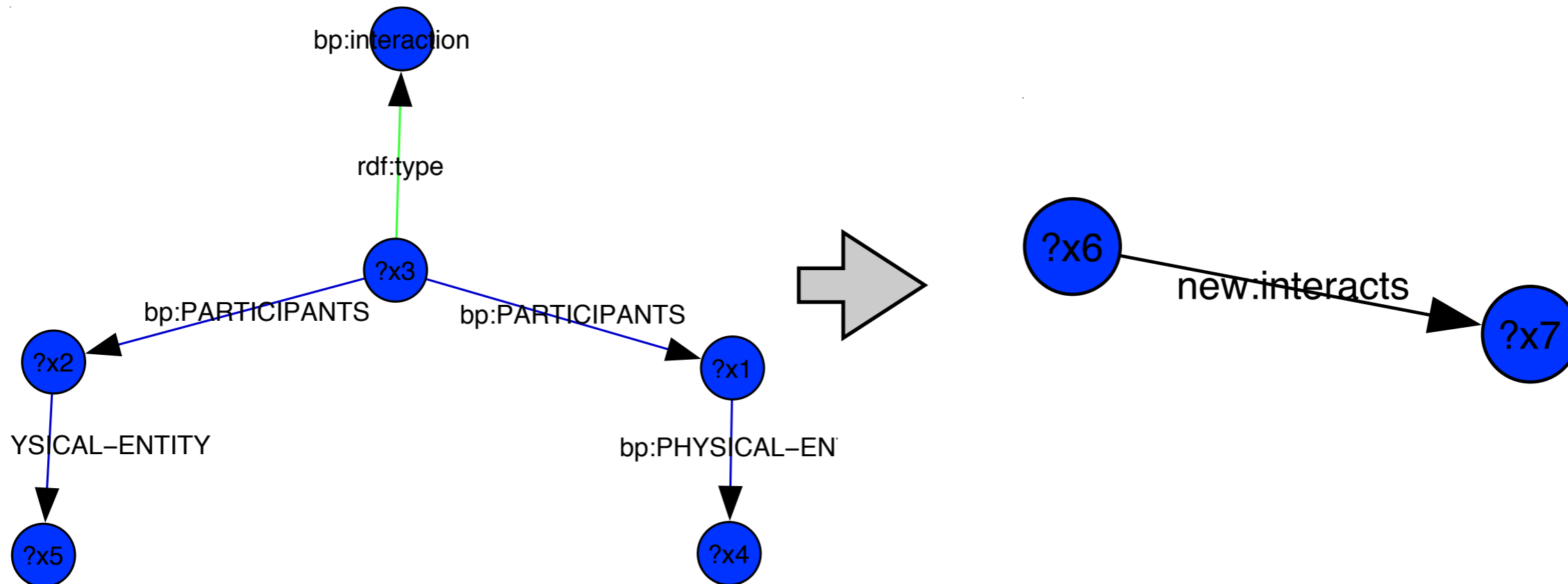


Queries

Reasoning



Reasoning



```
[Direct-interaction:
(?interactor new:dirInt ?p)
<-
(?x rdf:type bp:interaction)
(?x bp:PARTICIPANTS ?px)
(?px bp:PHYSICAL-ENTITY ?p)]
```

```
[Define-interaction:
(?pe1 new:interacts ?pe2)
<-
(?x rdf:type bp:interaction)
(?x new:dirInt ?pe1)
(?x new:dirInt ?pe2)]
```

RDFScape = Interface

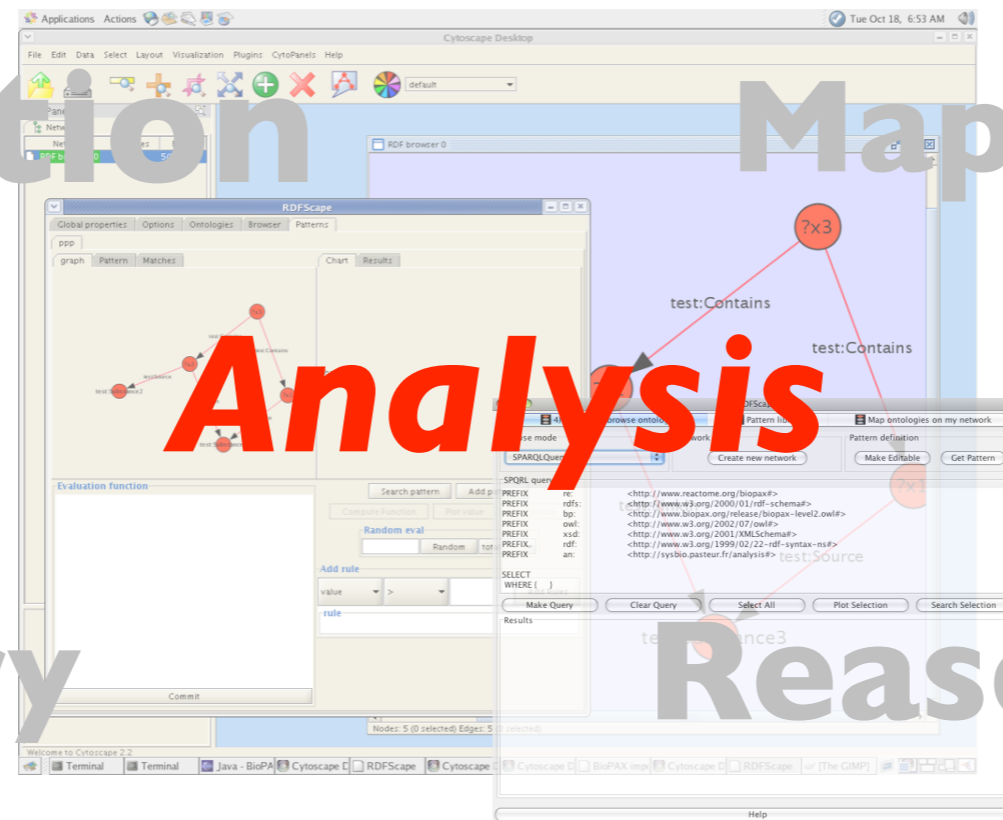
Inspection

Mapping

Analysis

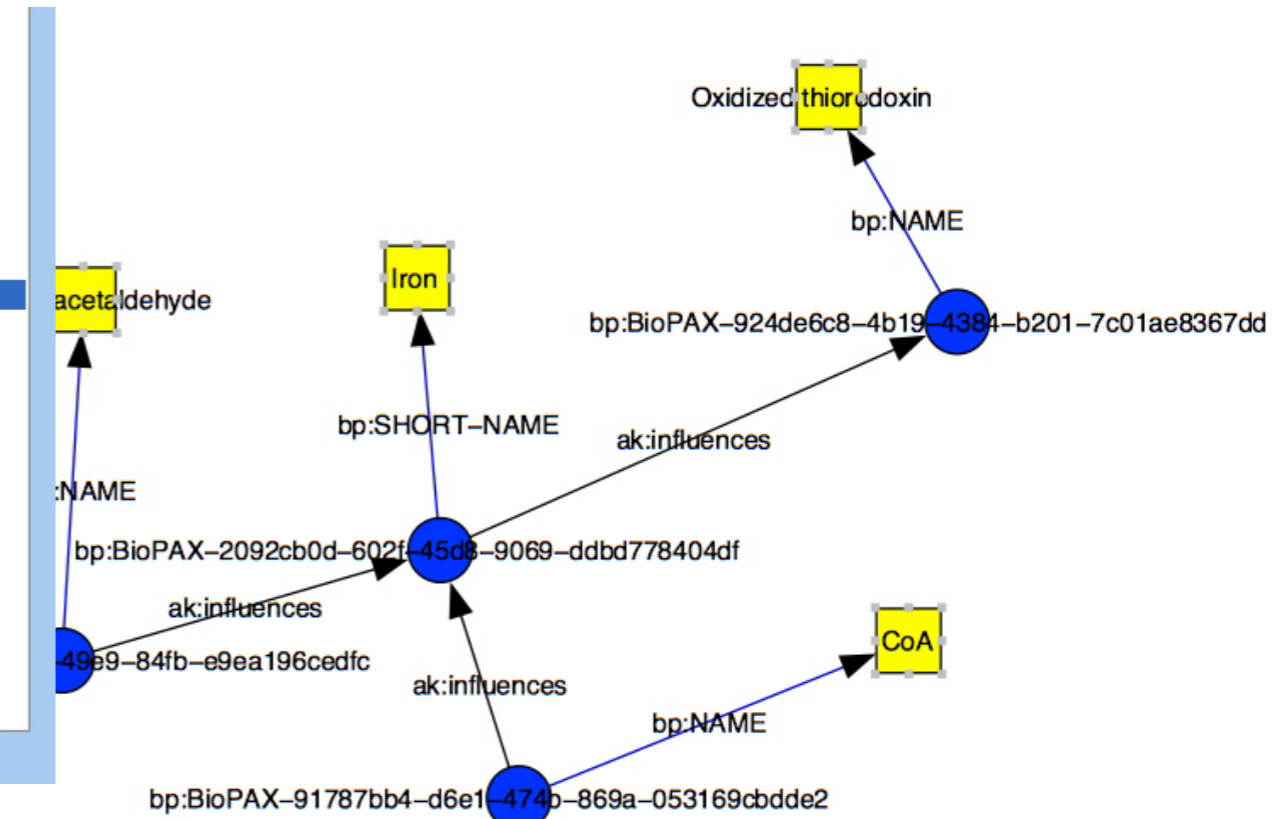
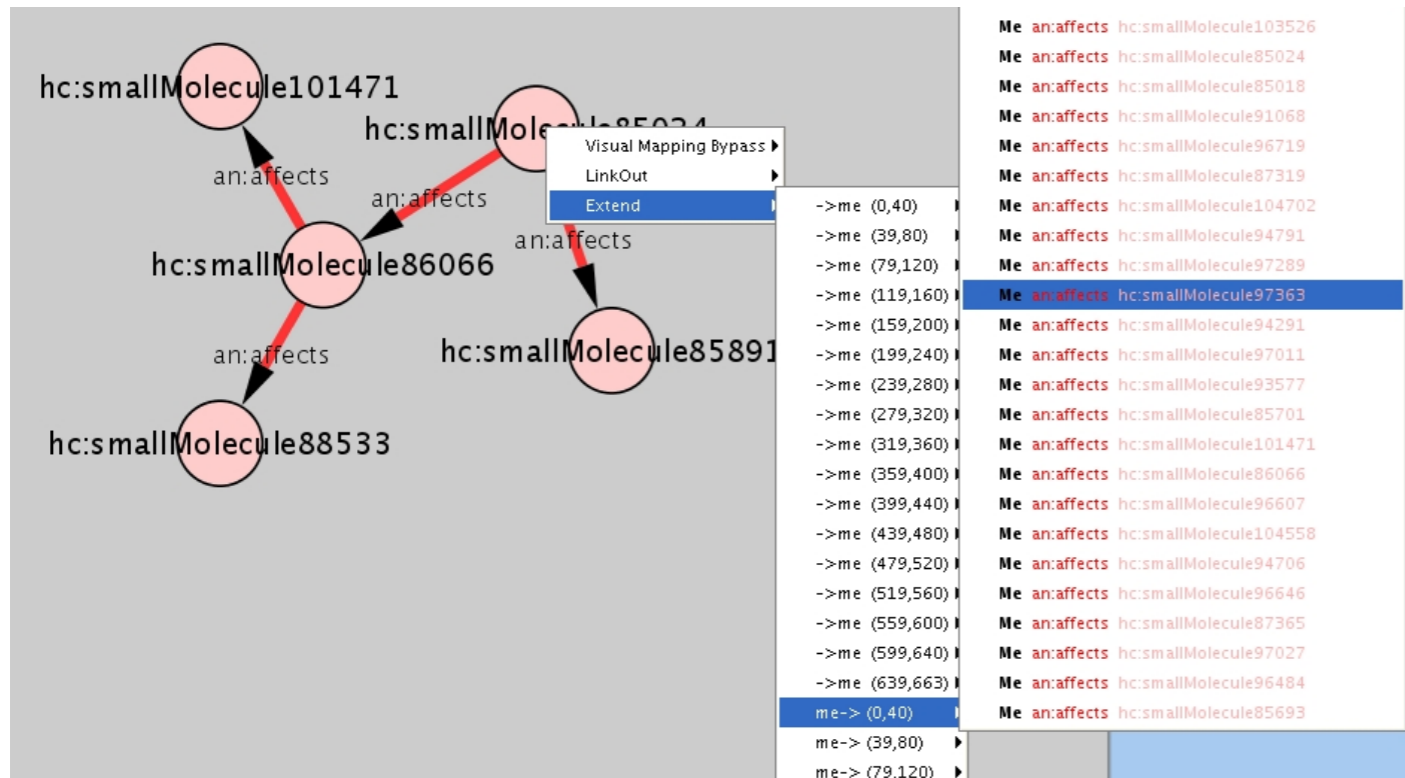
Query

Reasoning



Analysis

(Reasoning on pathways)



```
[influence: (?x ak:influences ?y) <- (?p1 rdf:type
bp:biochemicalReaction)
(?p2 rdf:type bp:biochemicalReaction)
(?p1 bp:RIGHT ?k1)(?k1 bp:PHYSICAL-ENTITY ?k)
(?p2 bp:LEFT ?k2)(?k2 bp:PHYSICAL-ENTITY ?k)
(?p1 bp:LEFT ?k3)(?k3 bp:PHYSICAL-ENTITY ?x)
(?p2 bp:RIGHT ?k4)(?k4 bp:PHYSICAL-ENTITY ?y) ]
```

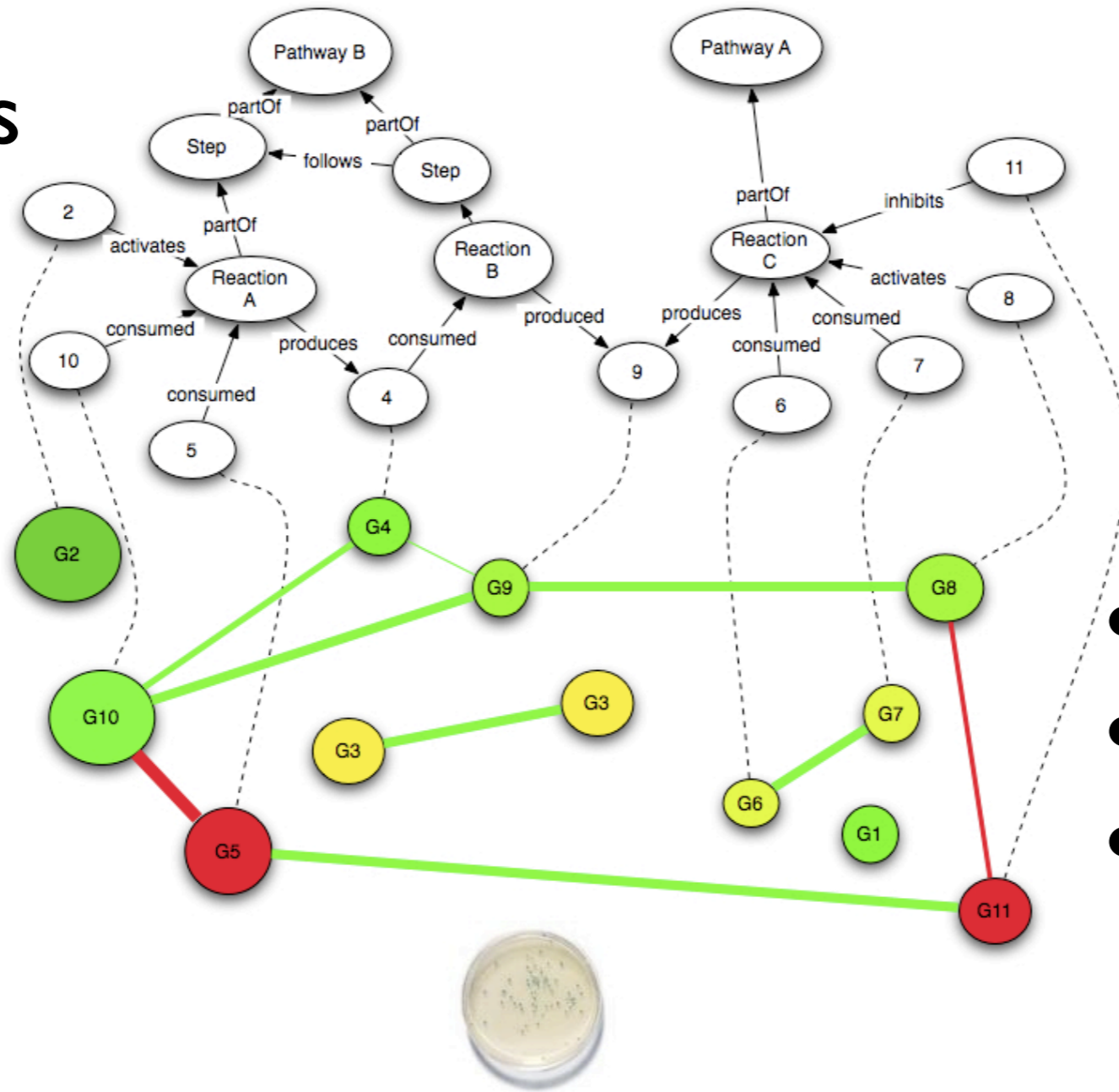
View of pathways as an influence graph

inference rules:
definition of "influence"

Analysis

(Ontologies and data)

- Ontologies
- General
- A-priori

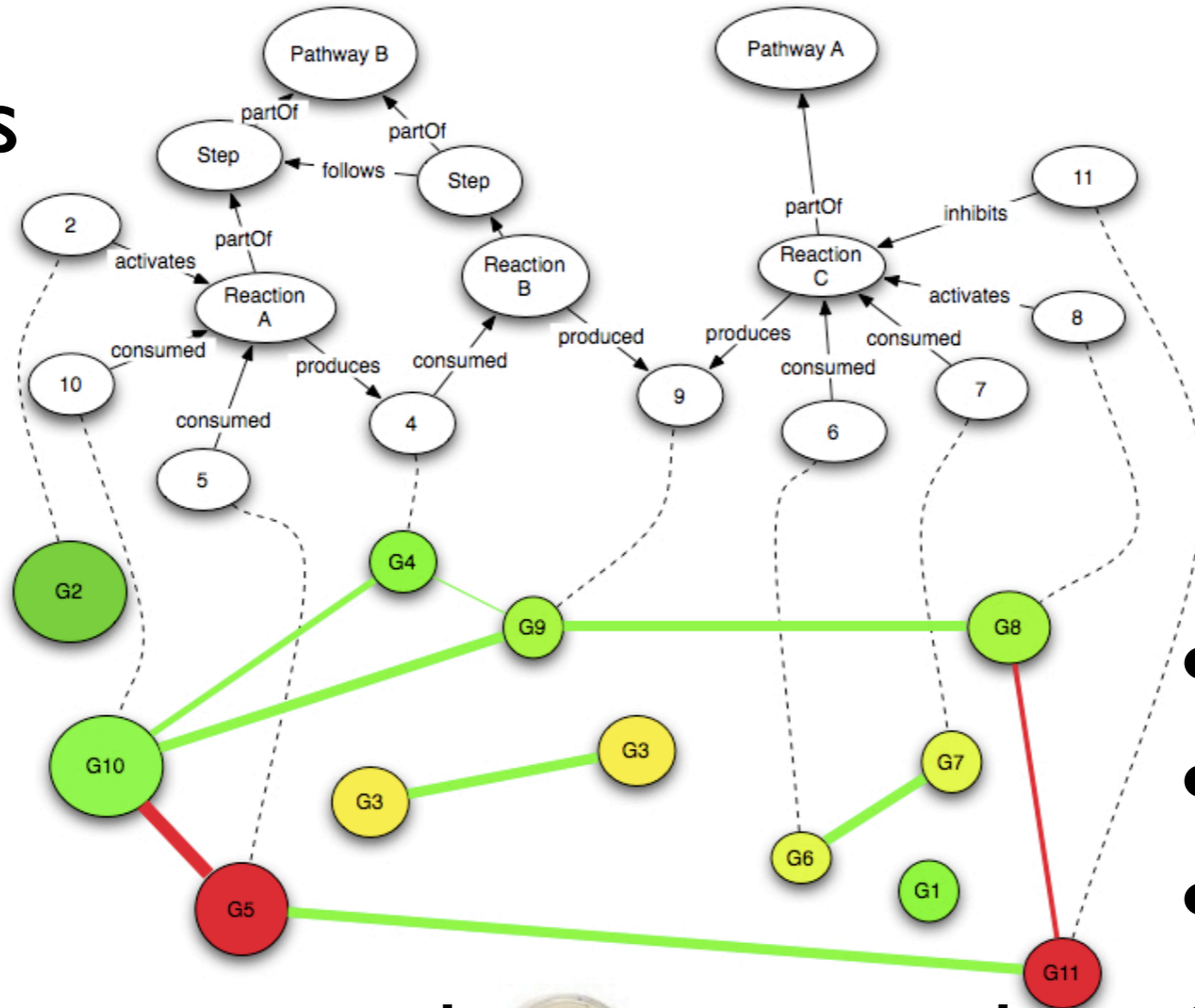


- Data
- Specific
- A-posteriori

Analysis

(Ontologies and data)

- Ontologies
- General
- A-priori

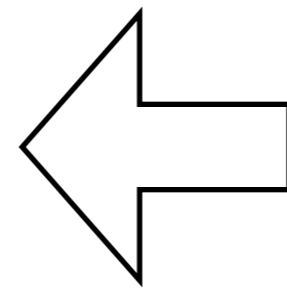
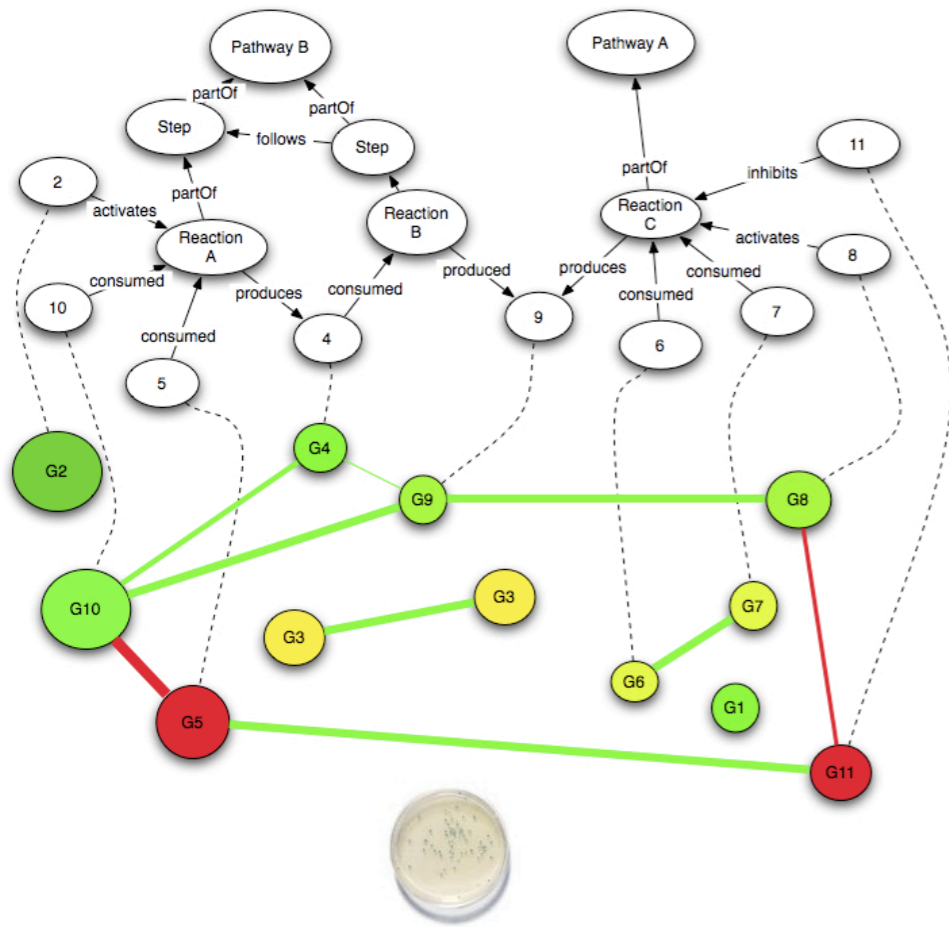


- Data
- Specific
- A-posteriori

The user open a correlation network in Cytoscape, and this is connected (through RDFScope) to ontologies

Analysis

(Ontologies and data)



Defining
the
mapping

Analysis

(Queries on ontologies and data)

The screenshot shows the RDFScope web application interface. At the top, there are navigation tabs: "4) Query and browse ontologies" (selected), "Pattern library", and "Map ontologies on my network". Below these are steps: "1) Select an analysis type!", "2) Load ontologies", and "3) (optional) configure options".

The interface is divided into three main sections:

- Browse mode:** A dropdown menu showing "SPARQLQuery".
- Network:** A "Create new network" button.
- Pattern definition:** "Make Editable" and "Get Pattern" buttons.

The **SPQRL query** section contains the following query:

```
PREFIX def: <http://www.leafbioscience.com/ontologies/test1#>
PREFIX ns0: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX ns1: <http://www.w3.org/2001/XMLSchema#>
PREFIX ns2: <http://www.w3.org/2002/07/owl#>
PREFIX ns3: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX ns4: <http://www.daml.org/2001/03/daml+oil#>
PREFIX n4: <http://rdfscape/network4#>

SELECT ?x ?relation ?y ?diffX ?stdvY
WHERE { ?x def:follows ?y .
       ?x n4:diff ?diffX .
       ?y n4:stdv ?stdvY .
       FILTER( ?diffX ) .
       FILTER( ?stdvY > 0.2 ) }
```

Below the query are buttons: "Make Query" (highlighted), "Clear Query", "Select All", "Plot Selection", and "Search Selection".

The **Results** section shows a table with the following data:

x	relation	y	diffX	stdvY
def:Peak3		def:Peak2	true	0.25
def:Peak2		def:Peak1	true	0.29

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Analysis

(Queries on ontologies and data)

All possible relations (in the **ontology**) between $?x$ and $?y$ (in the a network)

PREFIX def: <http://www.learbioscience.com/ontologies/test1#>
PREFIX s0: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX s1: <http://www.w3.org/2001/XMLSchema#>
PREFIX s2: <http://www.w3.org/2002/07/owl#>
PREFIX s3: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX n4: <http://www.daml.org/2001/03/daml+oil#>
PREFIX n5: <http://rdfscape/network4#>

SELECT ?x ?relation ?y ?diffX ?stdvY
WHERE { ?x def:follows ?y .
?x n4:diff ?diffX .
?y n4:stdv ?stdvY .
FILTER(?diffX) .
FILTER (?stdvY >0.2) }

Make Query

Clear Query

Select All

Plot Selection

Search Selection

Results

x	relation	y	diffX	stdvY
def:Peak3		def:Peak2	true	0.25
def:Peak2		def:Peak1	true	0.29

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Analysis

(Queries on ontologies and data)

All possible relations (in the **ontology**) between $?x$ and $?y$ (in the a network)

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PREFIX s0: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX s1: <http://www.w3.org/2001/XMLSchema#>
PREFIX s2: <http://www.w3.org/2002/07/owl#>
PREFIX s3: <http://www.w3.org/1999/02/22/rdf-syntax-ns#>
PREFIX s4: <http://www.daml.org/2001/07/swadlow/terms#>
PREFIX s5: <http://rdfscape/network#>
```

```
SELECT ?x ?relation ?y ?diffX ?stdvY
WHERE { ?x def:follows ?y .
        ?x n4:diff ?diffX .
        ?y n4:stdv ?stdvY .
        FILTER( ?diffX ) .
        FILTER ( ?stdvY > 0.2 ) }
```

Such that $?y$ **follows** $?x$
(inferred)

Make Query

Clear Query

Select All

Plot Selection

Search Selection

Results

x	relation	y	diffX	stdvY
def:Peak3		def:Peak2	true	0.25
def:Peak2		def:Peak1	true	0.29

Analysis

(Queries on ontologies and data)

All possible relations (in the **ontology**) between $?x$ and $?y$ (in the a network)

```
PREFIX def: <http://www.pearbioscience.com/ontologies/test1#>
PREFIX s0: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX s1: <http://www.w3.org/2001/XMLSchema#>
PREFIX s2: <http://www.w3.org/2002/07/owl#>
PREFIX s3: <http://www.w3.org/1999/02/22/rdf-syntax-ns#>
PREFIX s4: <http://www.daml.org/2001/03/xmlschema-org#>
PREFIX s5: <http://rdfscape/network#>
```

Such that $?y$ **follows** $?x$ (inferred)

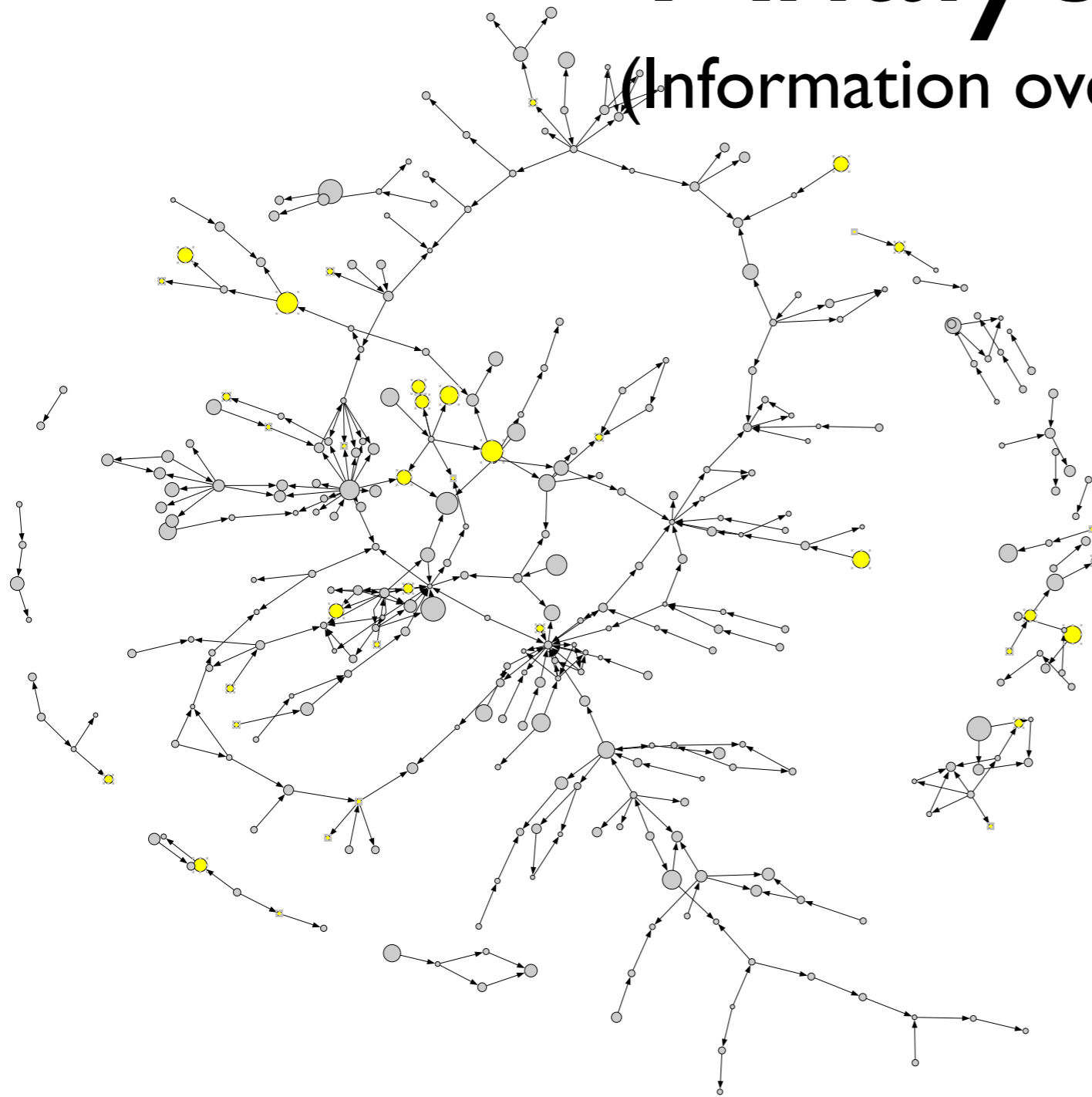
```
SELECT ?x ?relation ?y ?diffX ?stdvY
WHERE { ?x def:follows ?y .
        ?x n4:diff ?diffX .
        ?y n4:stdv ?stdvY .
        FILTER( ?diffX > 0.2 )
        FILTER ( ?stdvY > 0.2 ) }
```

Such $?x$ is **differentially expressed** and $?y$ has **variance** >0.2 (from data)

x	relation
def:Peak3	
def:Peak2	

Analysis

(Information overlay)



Selected elements in this p-p interaction graphs correspond to “controllers” in Kegg. The size of the nodes is proportional to the variance in gene expression

Analysis

VisHiC

(Using ontologies for data analysis)

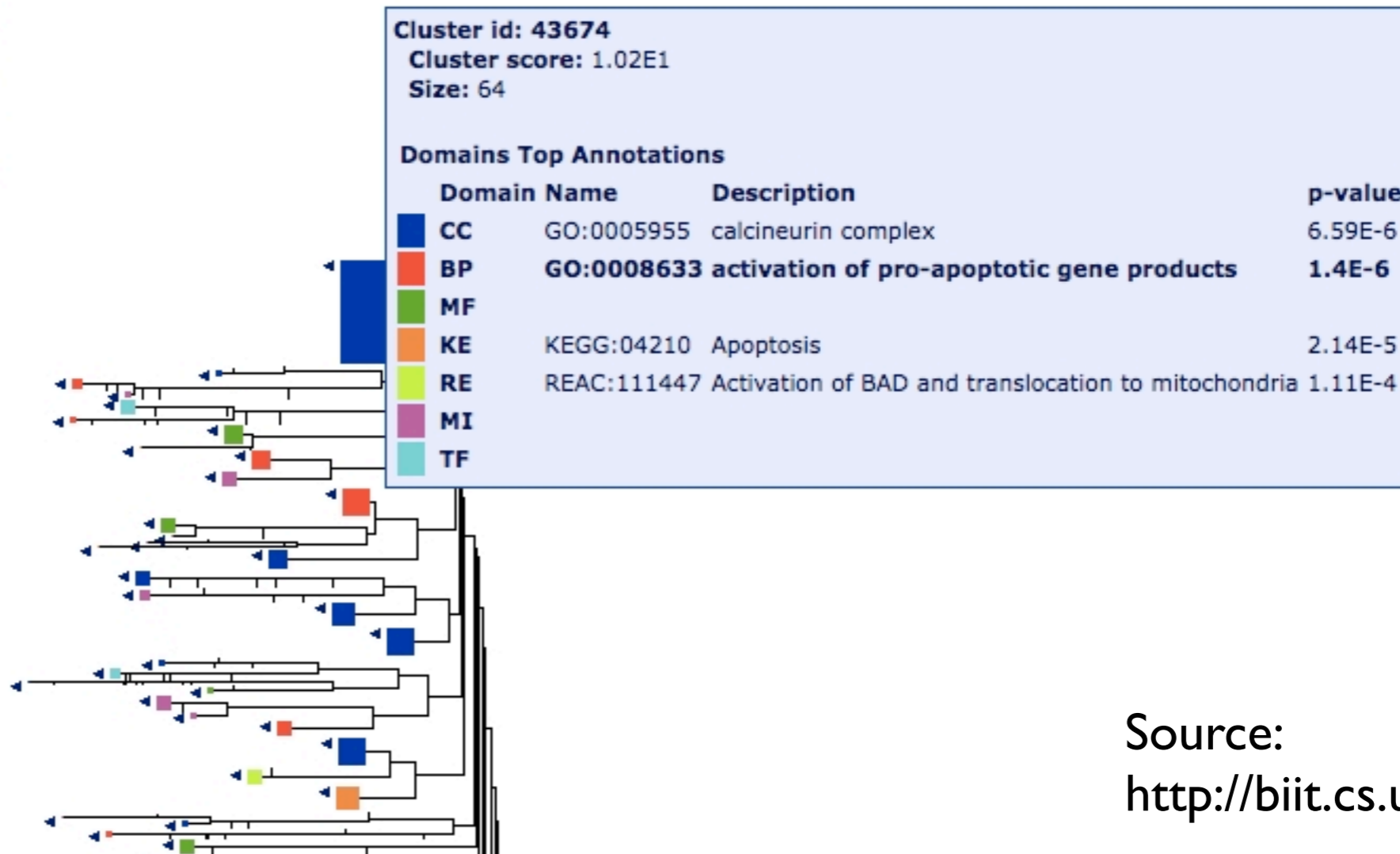
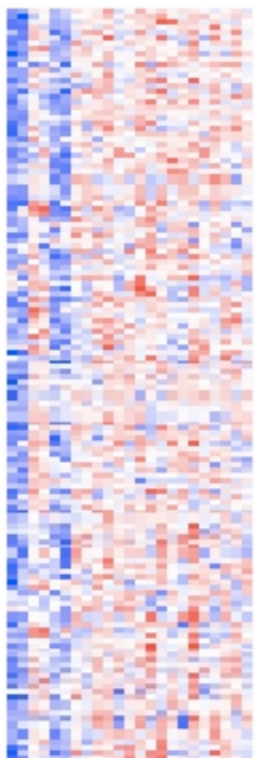
HOME >> DATASET ANALYSIS

HeLP

DATASET: GDS1023 HEMATOPOIETIC STEM CELL ENGRAFTMENT IN GOAT

Search for particular genes:

search!



Source:

<http://biit.cs.ut.ee/vishic/>

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Analysis

(Using ontologies for data analysis)

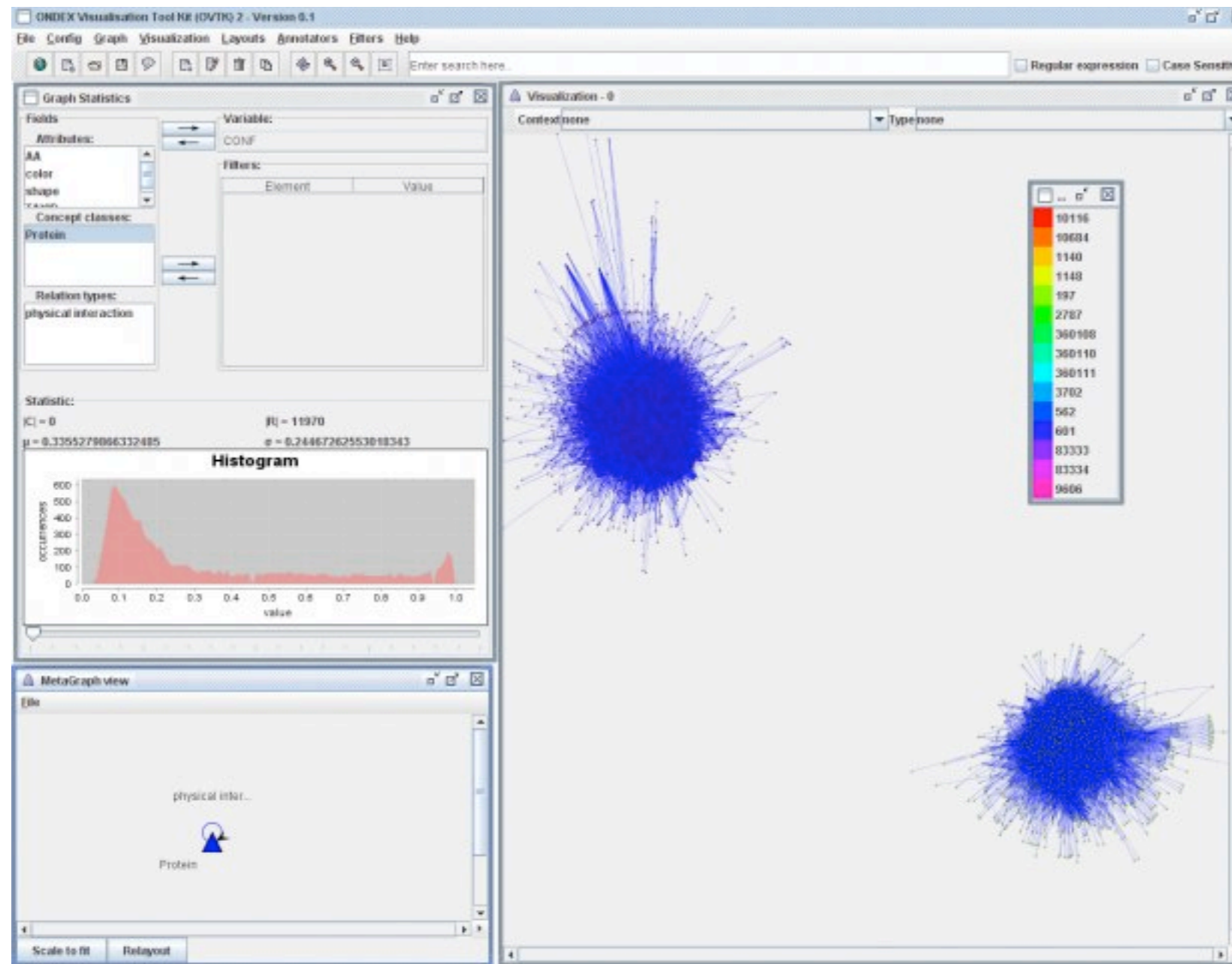
The screenshot displays the RDFScope application interface. On the left, a graph visualization shows a network of nodes and edges. The nodes include 'def:Pathway' (red oval), 'def:Gene' (red oval), and several unknown nodes (grey circles with '?'). Edges are labeled with 'ns3:type', 'def:contains', and 'def:follows'. Below the graph, the evaluation function is defined as:

$$f(?x3) = \frac{\text{SUM}(\text{corr}(?x4 \ ?x5))}{\text{NUM}(?x4) * \text{SUM}(\text{stdev}(?x4)) / \text{NUM}(?x4)}$$

The main window shows a 'Matches' table with columns 'x1' and 'x2'. The table lists various biological terms and their corresponding URIs. Below the table, there are controls for 'Search variables', 'Search patterns', 'Compute Funct...', 'Add rule', and 'Random eval'. The 'Compute Funct...' button is highlighted.

...	x1	x2	...	Pattern	Value	Pvalue
...	ns...	def:FakeInhibited	...	http://www.leaf...		
...	ns...	def:FakeActivated2	...	http://www.leaf...	0.158	
...	ns...	def:Peak3	...	http://www.leaf...	0.073	
...	ns...	def:Peak1	...	http://www.leaf...		
...	ns...	def:Pathway	...	http://www.leaf...		
...	ns...	def:FakeInhibited2	...	http://www.leaf...		
...	ns...	def:FakeActivated	...	http://www.leaf...	0.109	
...	ns...	def:Peak2	...	http://www.leaf...	0.18	

Analysis



Source:
<http://ondex.org/>

Can generic analysis tools be brought on the Semantic Web ?

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Conclusions

@Hackathon

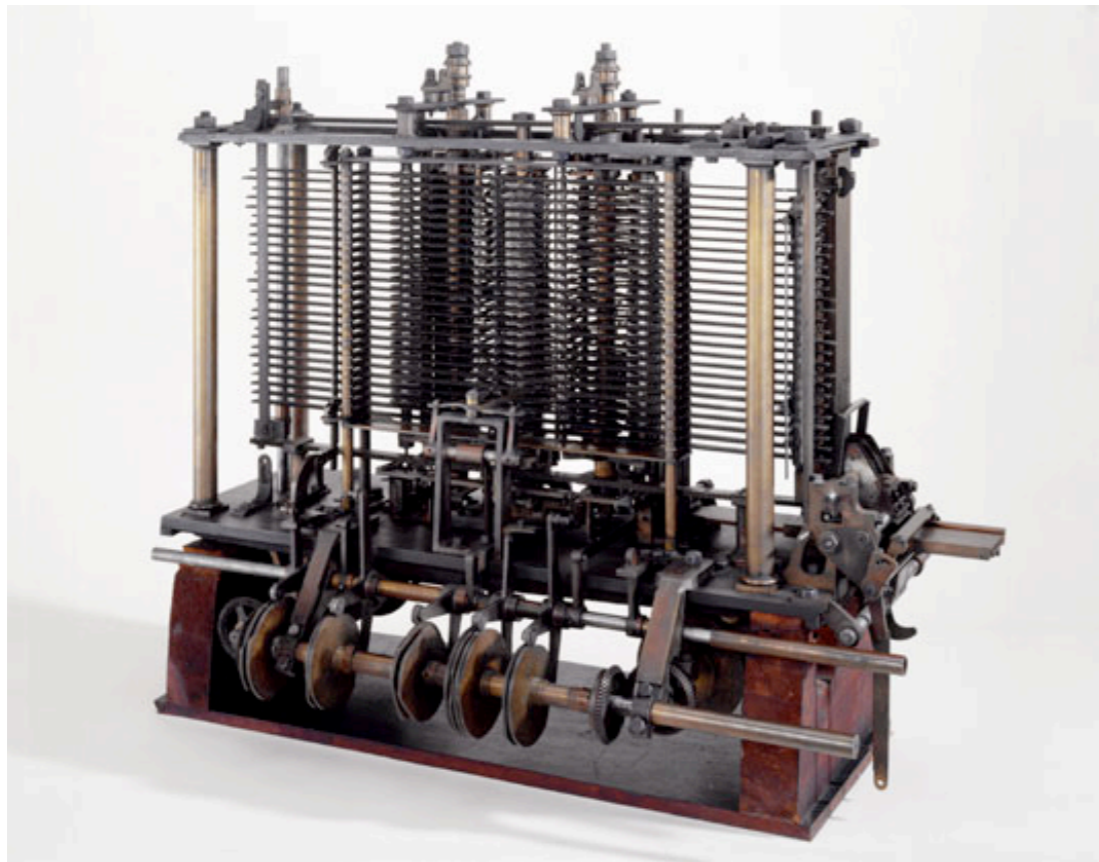
RDFScope:

Interaction+Query+Mapping+Reasoning+Analysis=
Interface

Conclusions @Hackathon

RDFScape:

Interaction+Query+Mapping+Reasoning+Analysis=
Interface



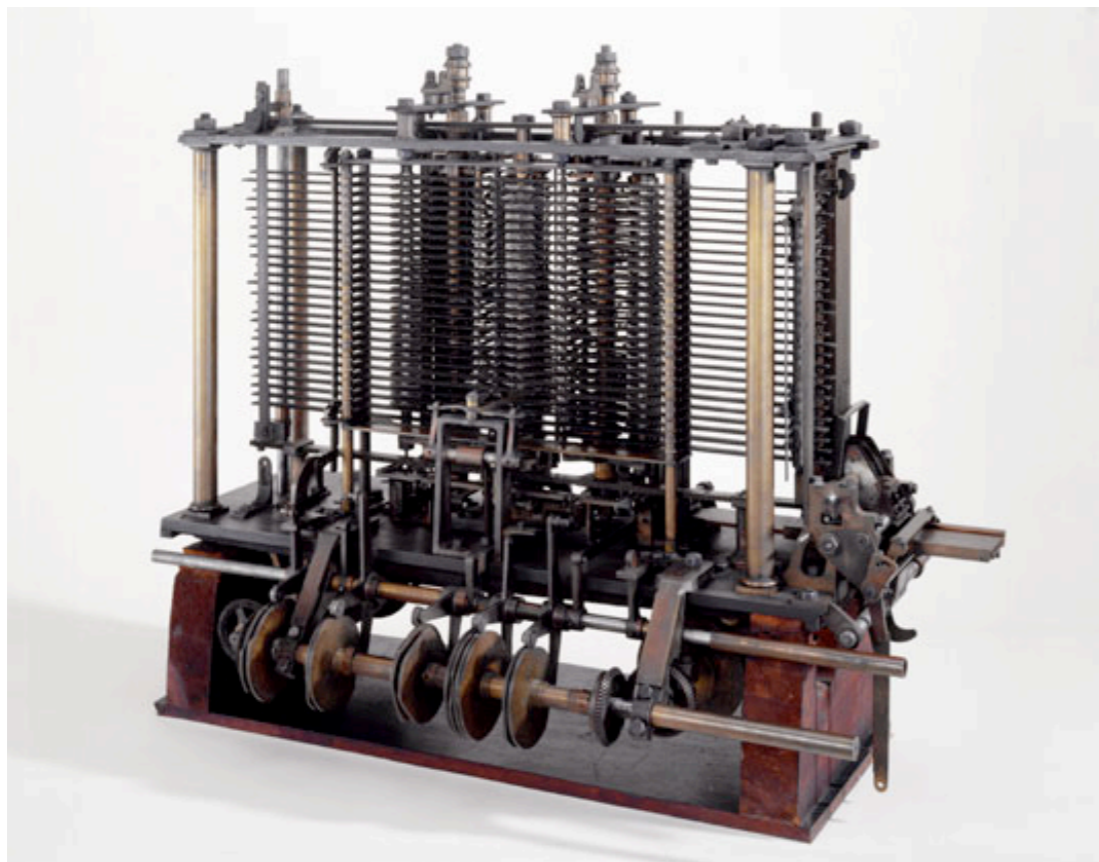
RDFScape today

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Conclusions @Hackathon

RDFScope:

Interaction+Query+Mapping+Reasoning+Analysis=
Interface



RDFScope today



RDFScope after the Hackaton

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References

RDFScape and network analysis (inference):

<http://www.biomedcentral.com/1471-2105/9/S4/S6/>

Semantic Web user interfaces (discussion):

<http://CEUR-WS.org/Vol-544/>

andrea.splendiani@bbsrc.ac.uk

The end

Thanks