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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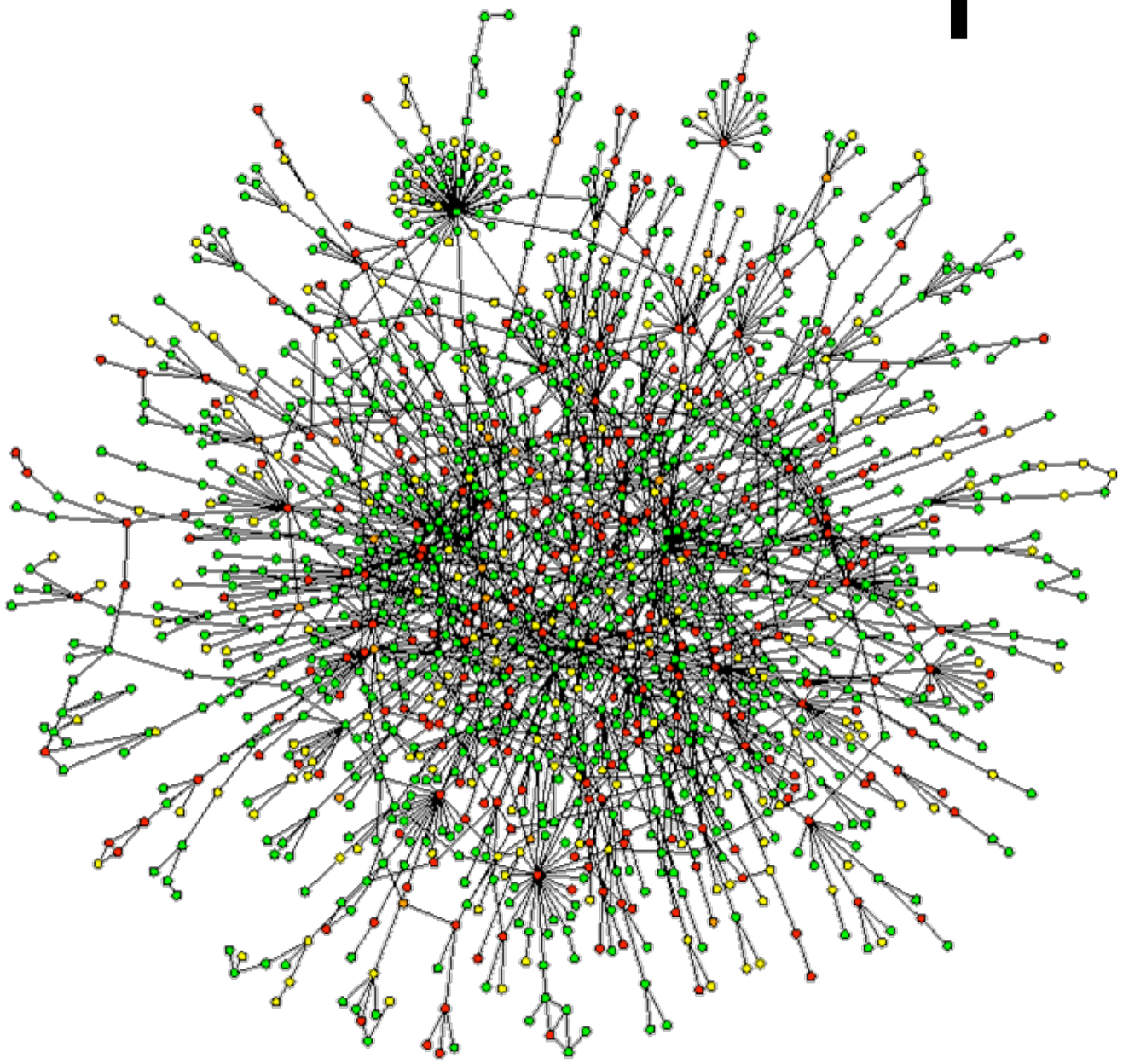
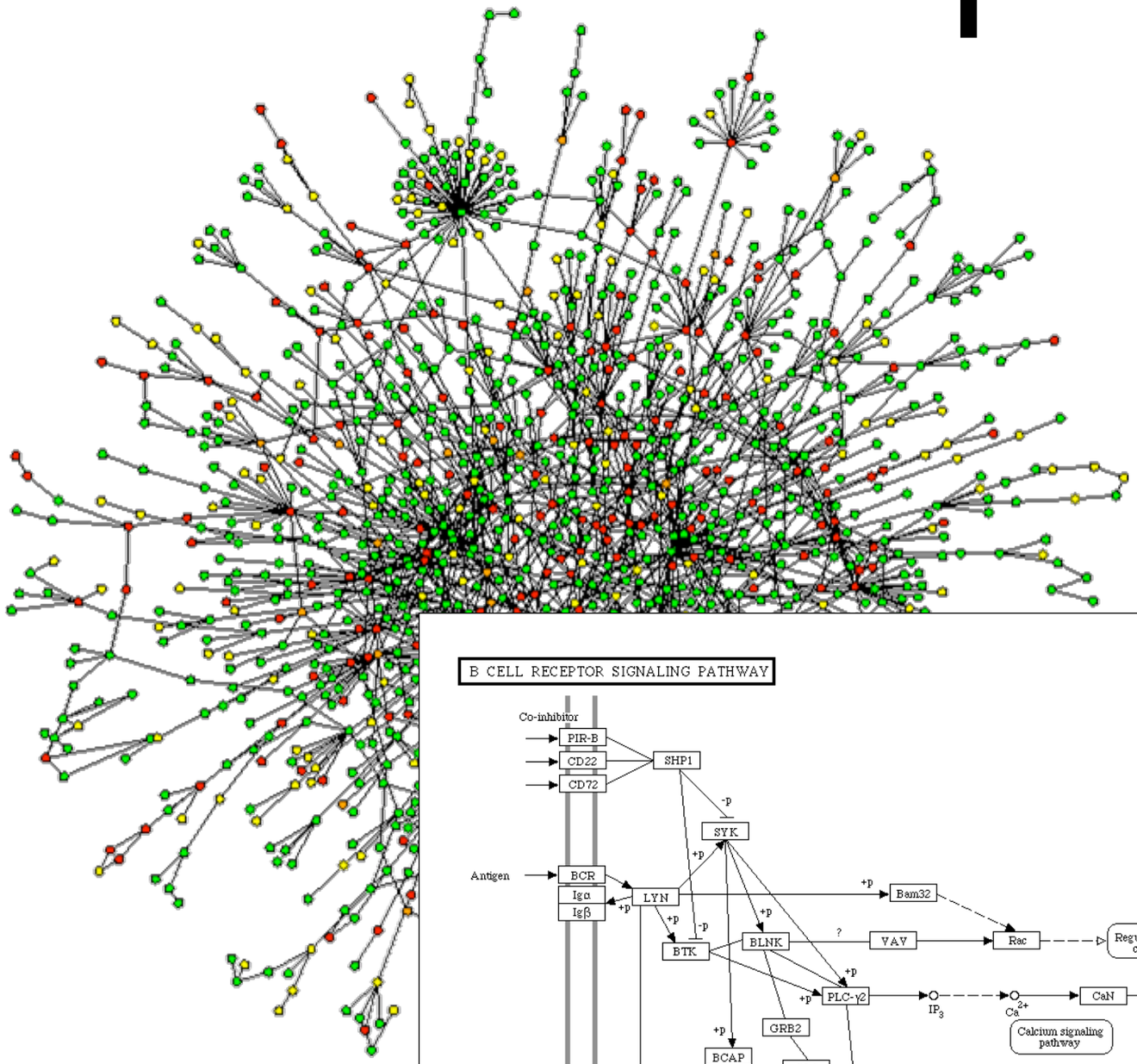
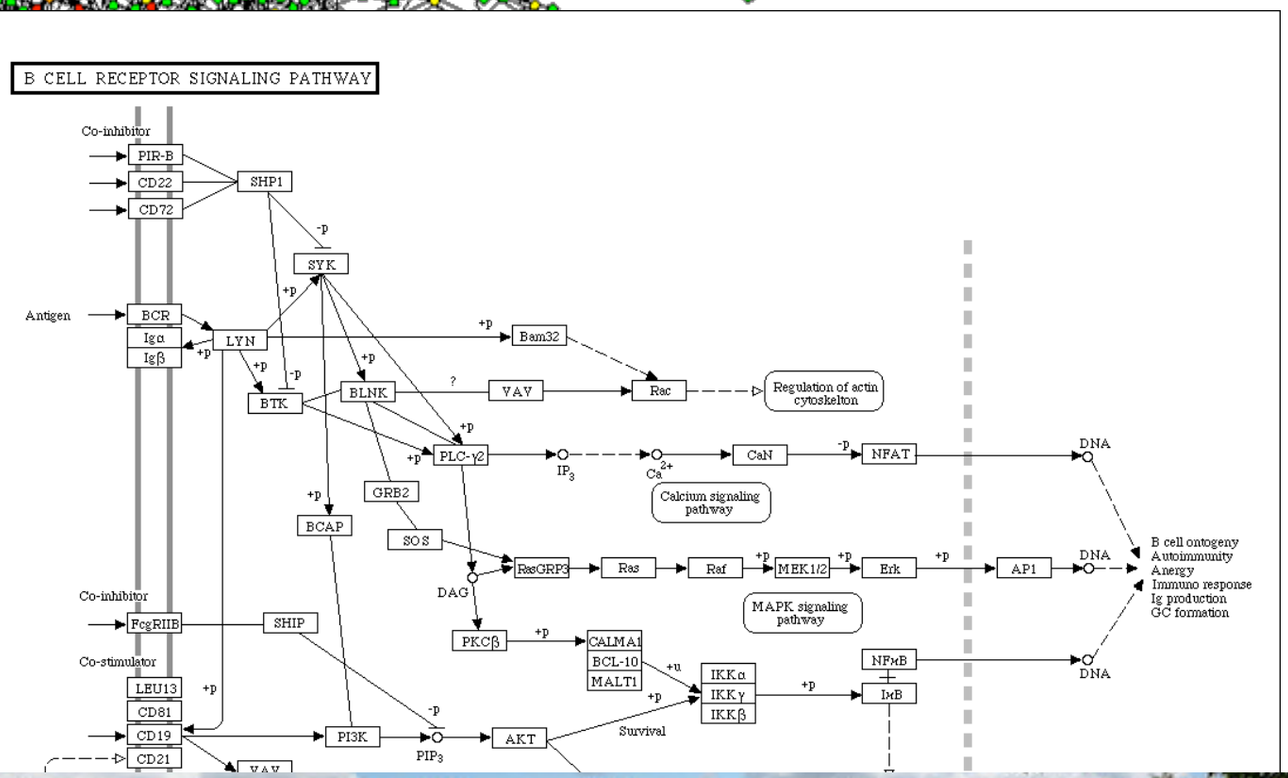
BioHackathon3 Symposium

The parts

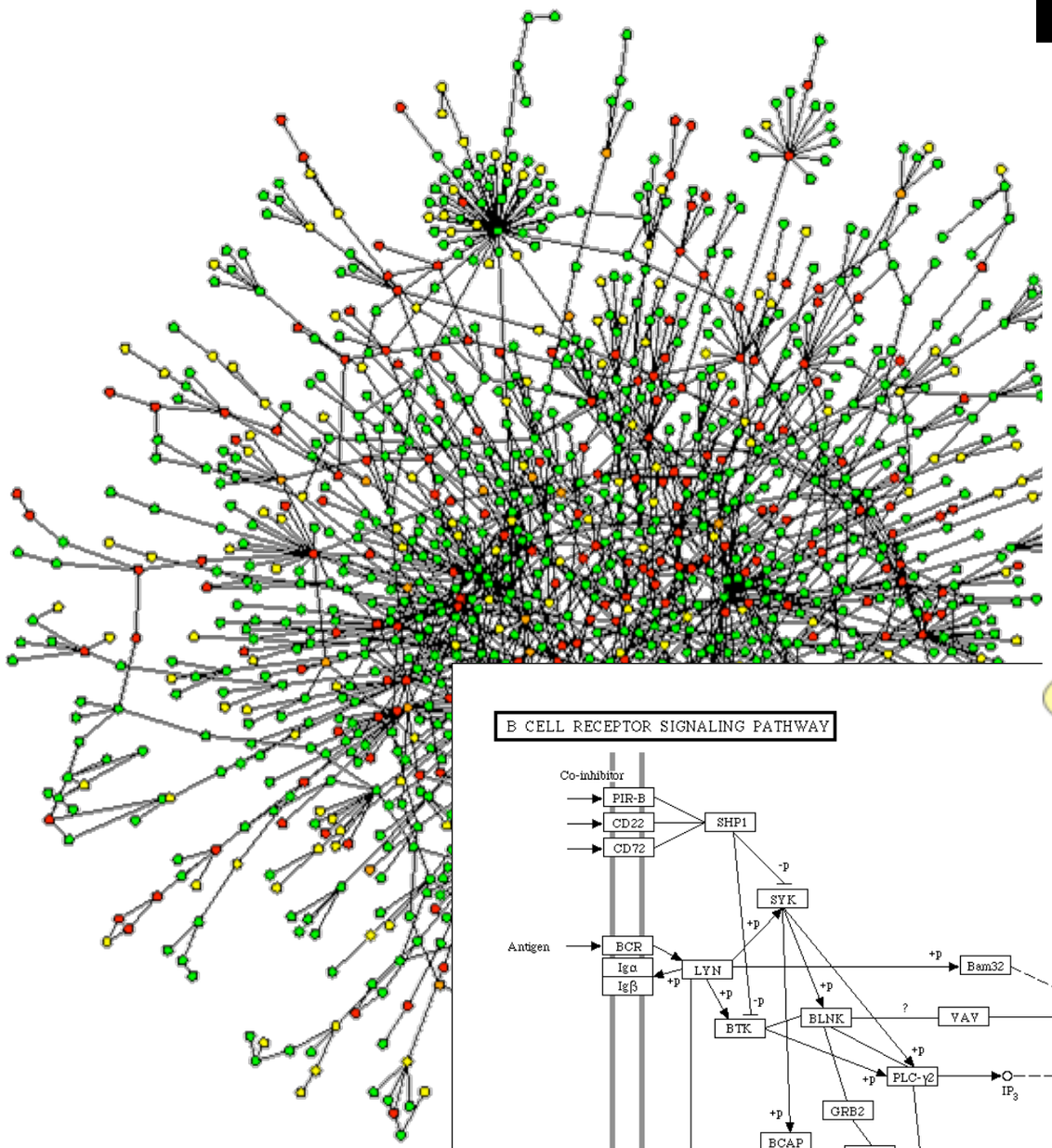


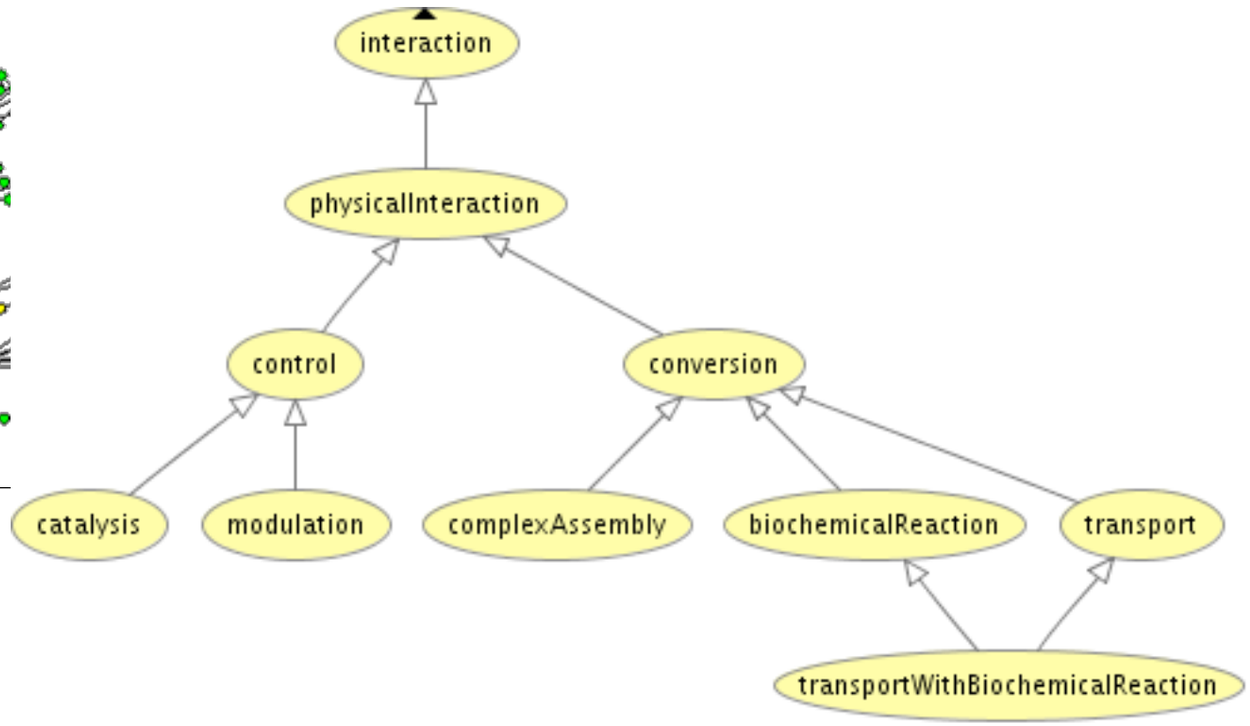
The parts




B CELL RECEPTOR SIGNALING PATHWAY
Co-inhibitor
PIR-B
CD22
CD72
SHP1
SYK
Antigen
BCR
Igα
Igβ
LYN
Bam32
BTK
BLNK
VAV
Rac
Regulation of actin cytoskelton
PLC-γ2
IP3
Ca2+
CaN
NFAT
DNA
Calcium signaling pathway
GRB2
BCAP
SOS
RasGRP3
Ras
Raf
MEK1/2
Erk
AP1
DAG
MAPK signaling pathway
B cell ontogeny
Autoimmunity
Anergy
Immuno response
Ig production
GC formation
Co-inhibitor
FcgRIIB
SHIP
PKCβ
CALMA1
BCL-10
MALT1
Co-stimulator
LEU13
CD81
CD19
CD21
PI3K
PIP3
AKT
Survival
IKKα
IKKγ
IKKβ
NFκB
IκB

The parts

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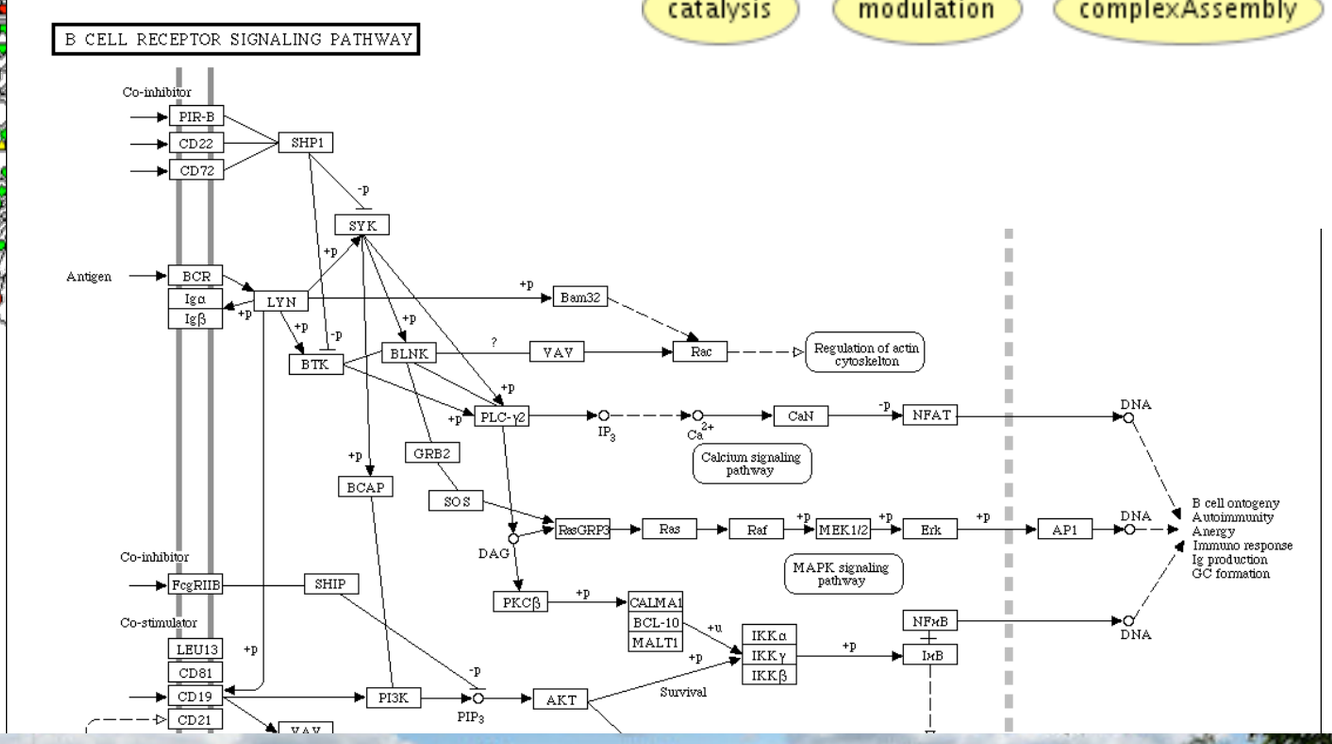
physicalInteraction
control
conversion
catalysis
modulation
complexAssembly
biochemicalReaction
transport
transportWithBiochemicalReaction


B CELL RECEPTOR SIGNALING PATHWAY
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Igβ
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Raf
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FcgRIIB
SHIP
PKCβ
CALMA1
BCL-10
MALT1
IKKα
IKKγ
IKKβ
NFκB
IκB
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LEU13
CD81
CD19
CD21
PI3K
PIP3
AKT
Survival


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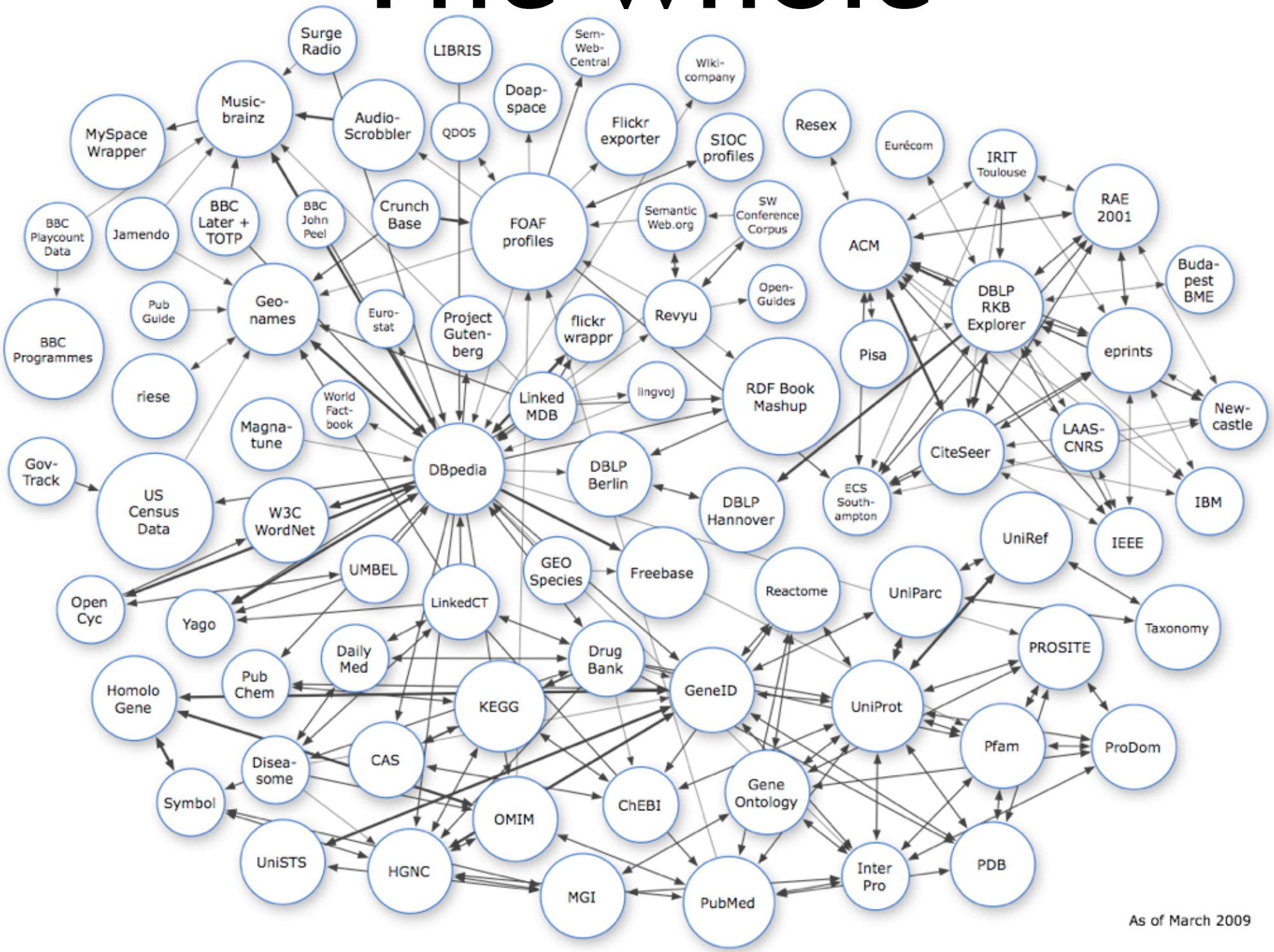
The whole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LIBRIS
Sem-Web-Central
Wiki-company
Music-brainz
Audio-Scrobbler
Doap-space
Flickr exporter
SIOC profiles
Resex
Eurécom
IRIT Toulouse
MySpace Wrapper
QDOS
BBC Playcount Data
Jamendo
BBC Later + TOTP
BBC John Peel
Crunch Base
FOAF profiles
Semantic Web.org
SW Conference Corpus
ACM
RAE 2001
Buda-pest BME
Pub Guide
Geo-names
Euro-stat
Project Guten-berg
flickr wrappr
Revyu
Open-Guides
DBLP RKB Explorer
BBC Programmes
Pisa
eprints
riese
World Fact-book
Linked MDB
lingvoj
RDF Book Mashup
New-castle
Magna-tune
LAAS-CNRS
Gov-Track
DBpedia
DBLP Berlin
CiteSeer
US Census Data
W3C WordNet
DBLP Hannover
ECS South-ampton
IBM
UMBEL
GEO Species
Freebase
UniRef
IEEE
Open Cyc
LinkedCT
Reactome
UniParc
Taxonomy
Yago
Daily Med
Drug Bank
PROSITE
Homolo Gene
Pub Chem
KEGG
GeneID
UniProt
Pfam
ProDom
Disea-some
CAS
Gene Ontology
Symbol
OMIM
ChEBI
UniSTS
HGNC
Inter Pro
PDB
MGI
PubMed
As of March 2009


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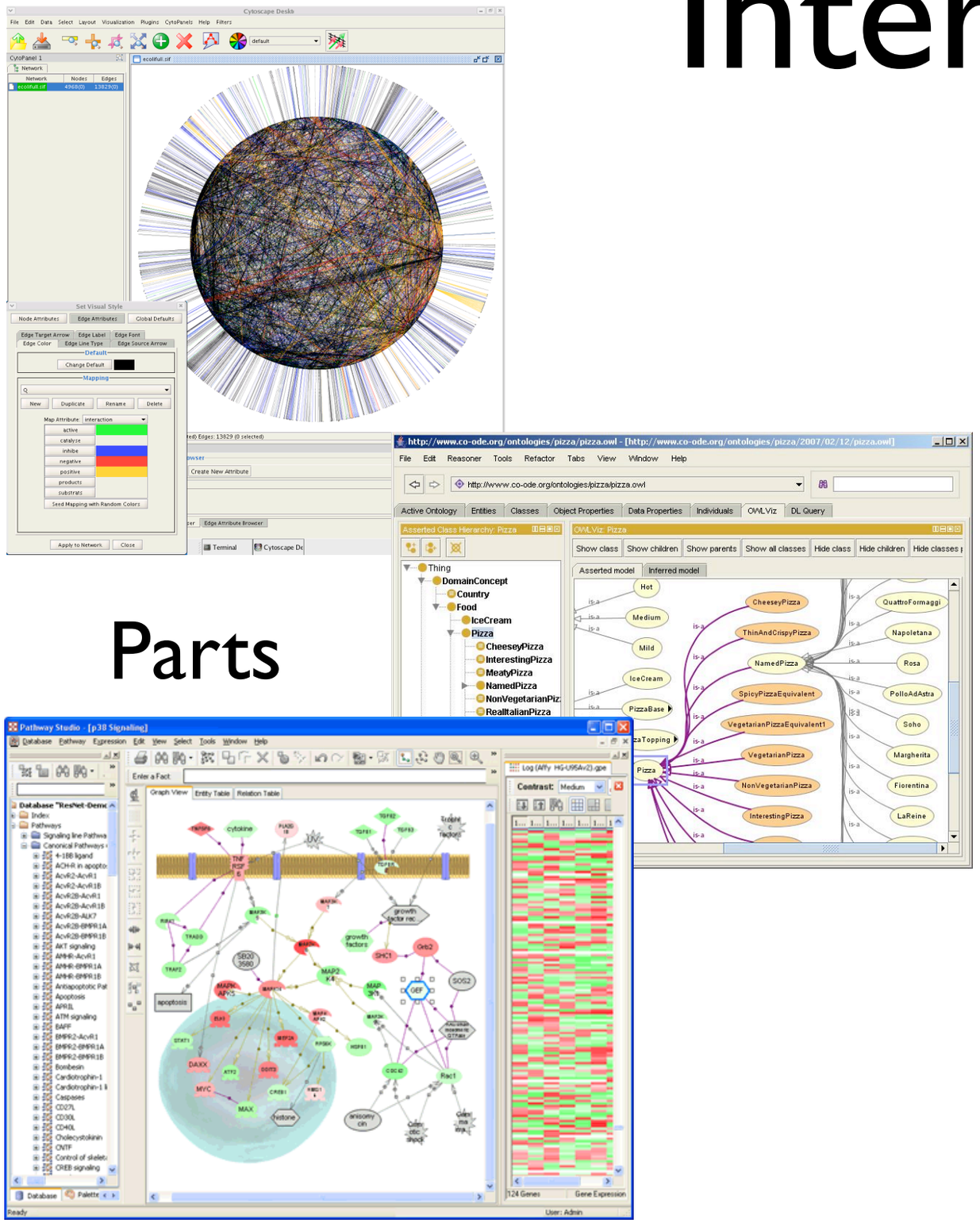
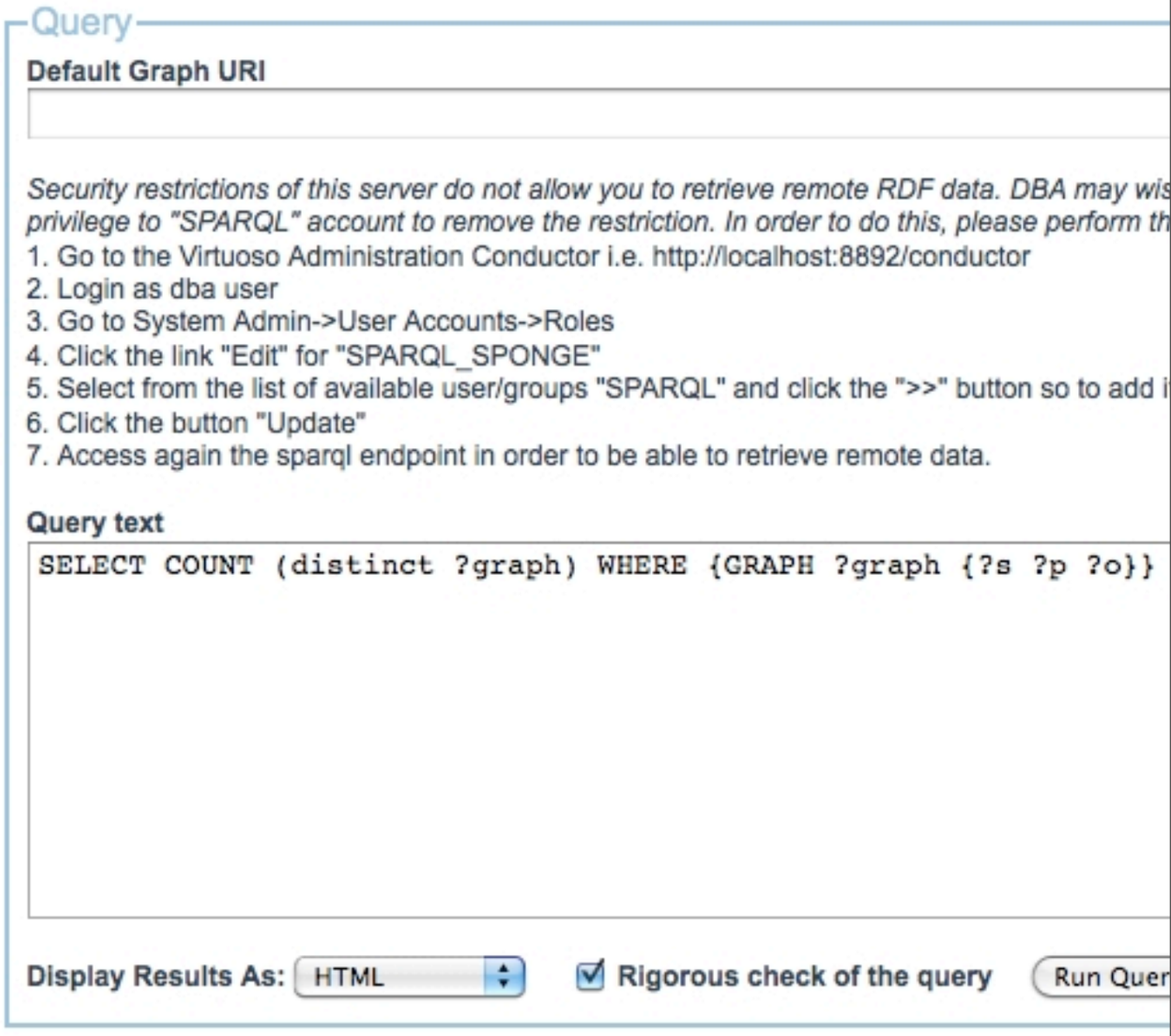
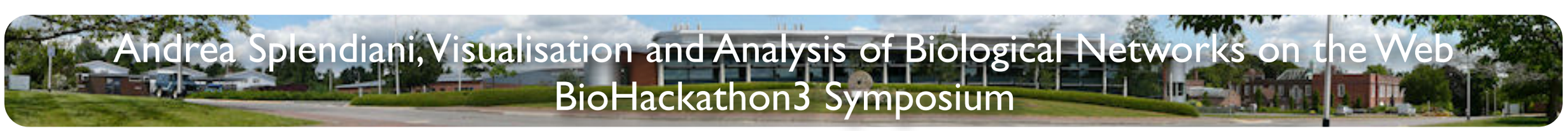
Interfaces

Parts

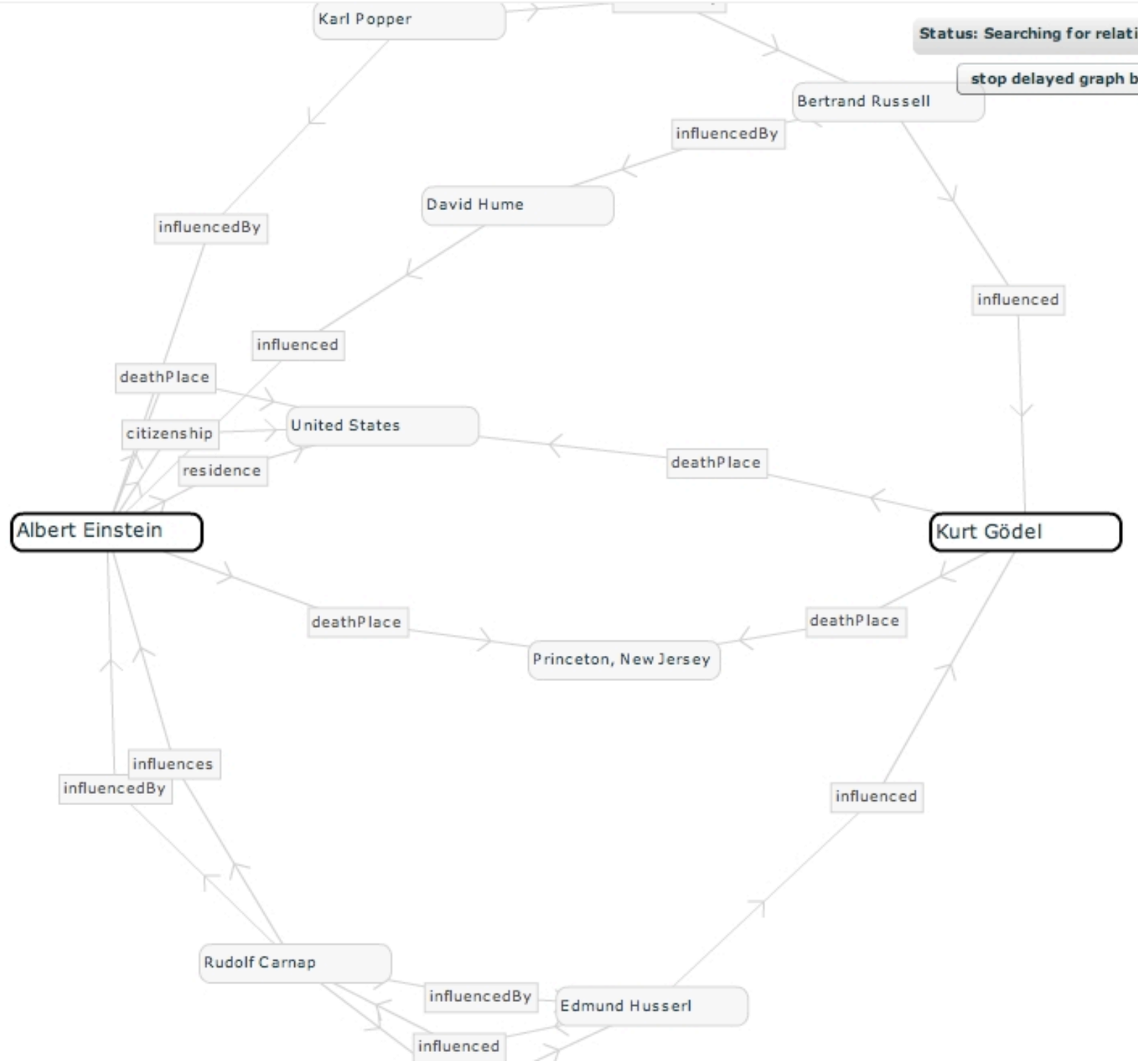


Whole



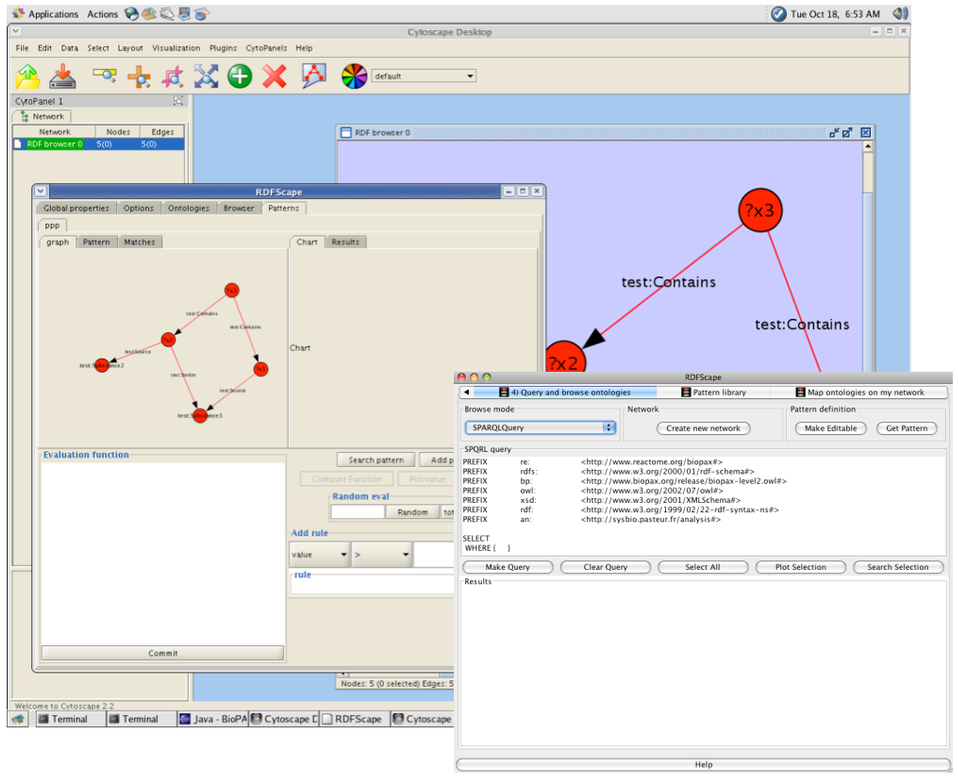


Interfaces



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

RDFScape


Applications Actions
Tue Oct 18, 6:53 AM
Cytoscape Desktop
File Edit Data Select Layout Visualization Plugins CytoPanels Help
default
CytoPanel 1
Network
Network Nodes Edges
RDF browser 0 5(0) 5(0)
RDF browser 0
RDFScape
Global properties Options Ontologies Browser Patterns
ppp
graph Pattern Matches
Chart Results
Chart
Evaluation function
Search pattern
Compute Function Plot value
Random eval
Random
Add rule
value >
rule
Commit
Nodes: 5 (0 selected) Edges: 5
Welcome to Cytoscape 2.2
Terminal Terminal Java - BioPA Cytoscape D RDFScape Cytoscape
?x3
test:Contains
test:Contains
?x2
RDFScape
4) Query and browse ontologies
Pattern library
Map ontologies on my network
Browse mode
SPARQLQuery
Network
Create new network
Pattern definition
Make Editable
Get Pattern
SPQRL query
PREFIX re: <http://www.reactome.org/biopax#>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX bp: <http://www.biopax.org/release/biopax-level2.owl#>
PREFIX owl: <http://www.w3.org/2002/07/owl#>
PREFIX xsd: <http://www.w3.org/2001/XMLSchema#>
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
PREFIX an: <http://sysbio.pasteur.fr/analysis#>
SELECT
WHERE { }
Make Query
Clear Query
Select All
Plot Selection
Search Selection
Results
Help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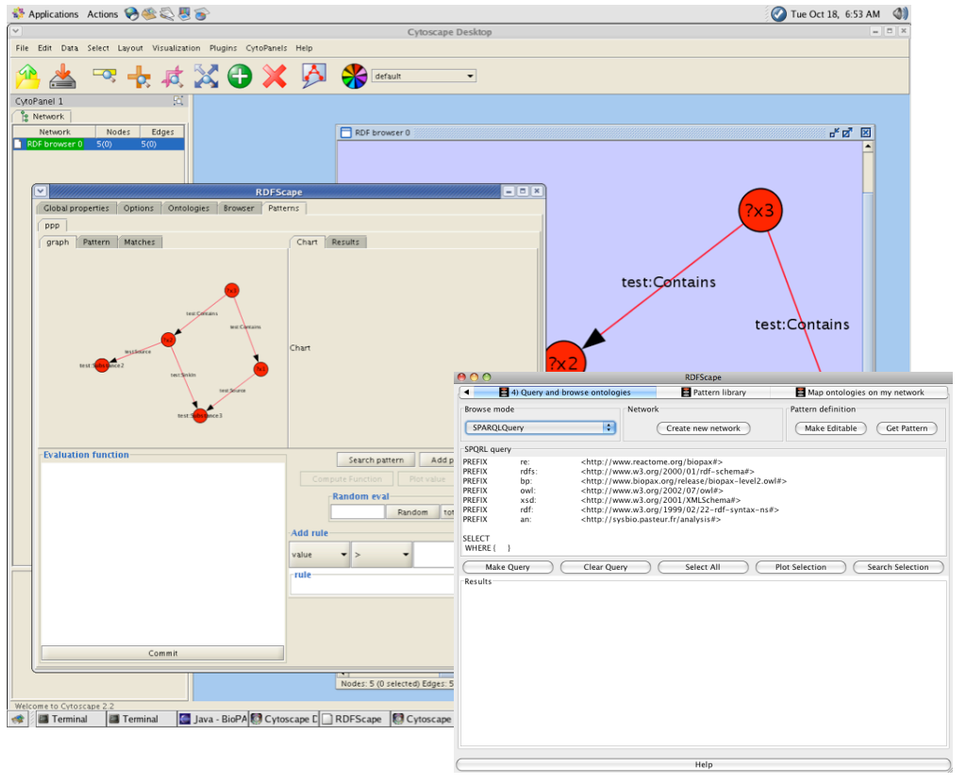
RDFScape = Interface

Using Cytoscape for interaction on the Semantic Web



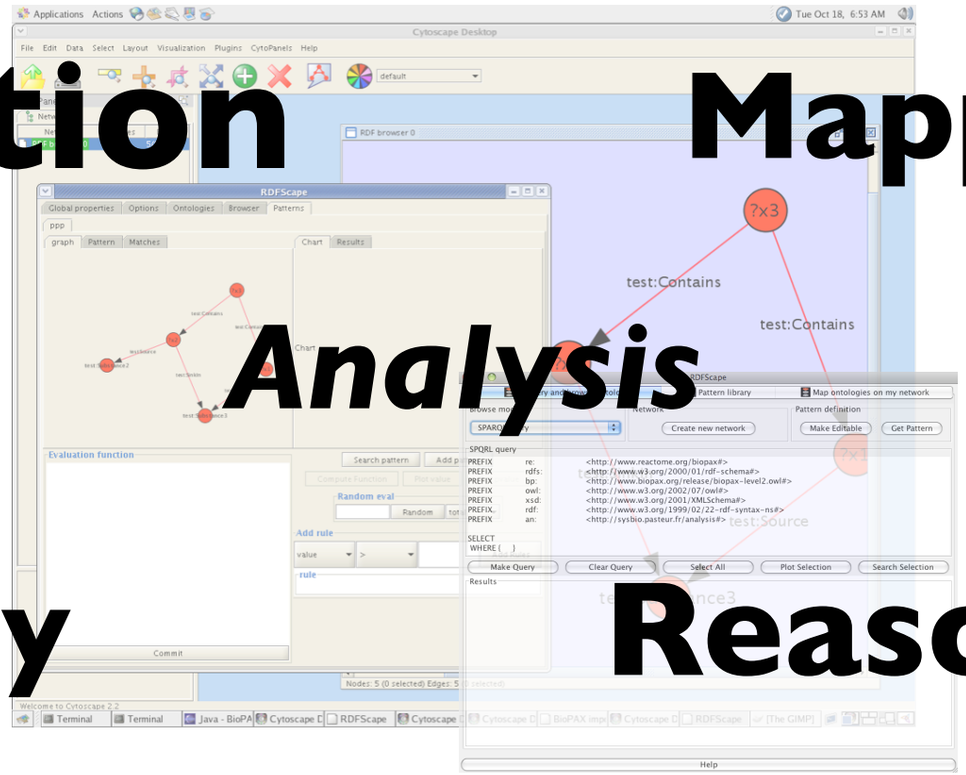
Using the Semantic Web for the analysis of networks in Cytoscape

RDFScape = Interface

Inspection **Mapping**

Analysis

Query **Reasoning**

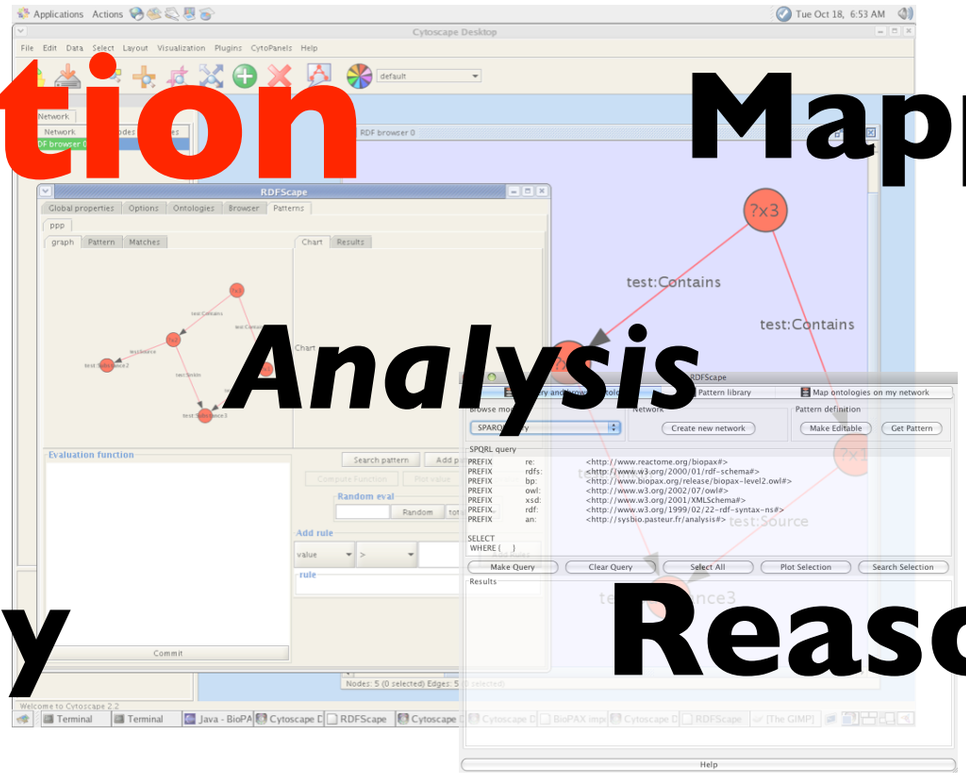


RDFScape = Interface

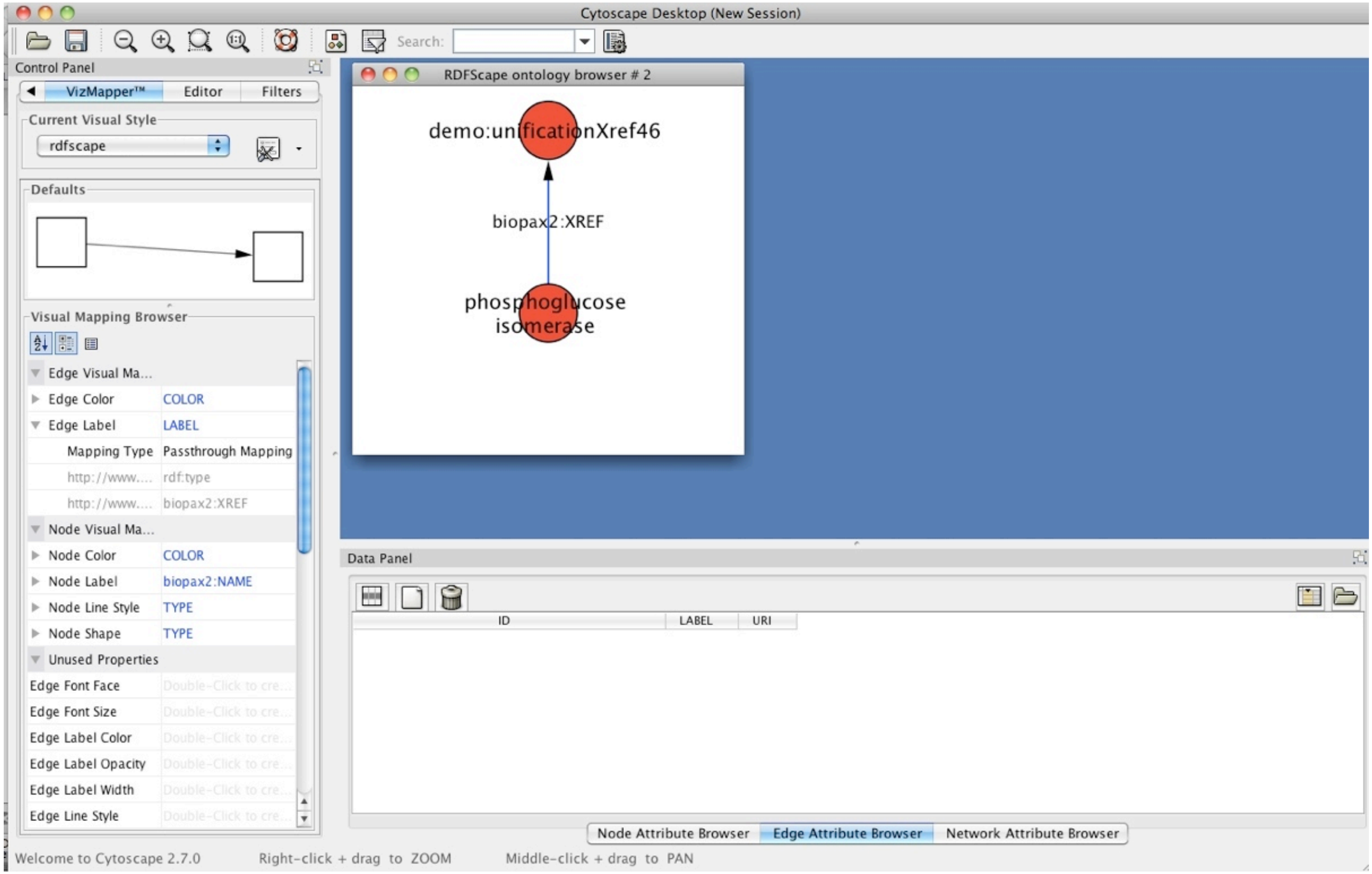
Inspection **Mapping**

Analysis

Query **Reasoning**



Inspection


Cytoscape Desktop (New Session)
Search:
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
Edge Font Size
Edge Label Color
Edge Label Opacity
Edge Label Width
Edge Line Style
RDFScape ontology browser # 2
demo:unificationXref46
biopax2:XREF
phosphoglucose
isomerase
Data Panel
ID
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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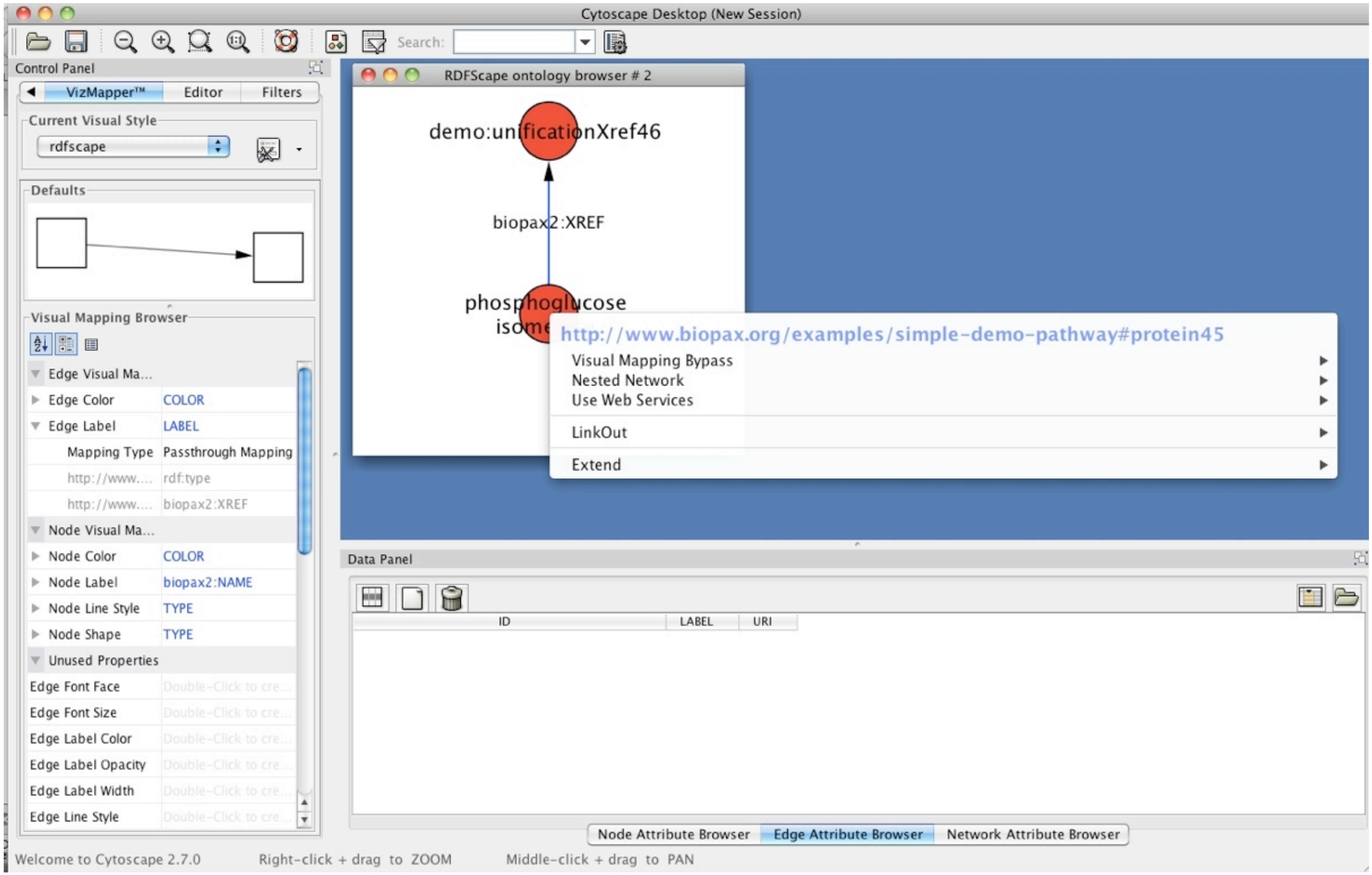
Inspection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Mapping Type
Passthrough Mapping
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rdf:type
http://www....
biopax2:XREF
Node Visual Ma...
Node Color
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Node Label
biopax2:NAME
Node Line Style
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Edge Label Opacity
Edge Label Width
Edge Line Style
RDFScape ontology browser # 2
demo:unificationXref46
biopax2:XREF
phosphoglucose
isome
http://www.biopax.org/examples/simple-demo-pathway#protein45
Visual Mapping Bypass
Nested Network
Use Web Services
LinkOut
Extend
Data Panel
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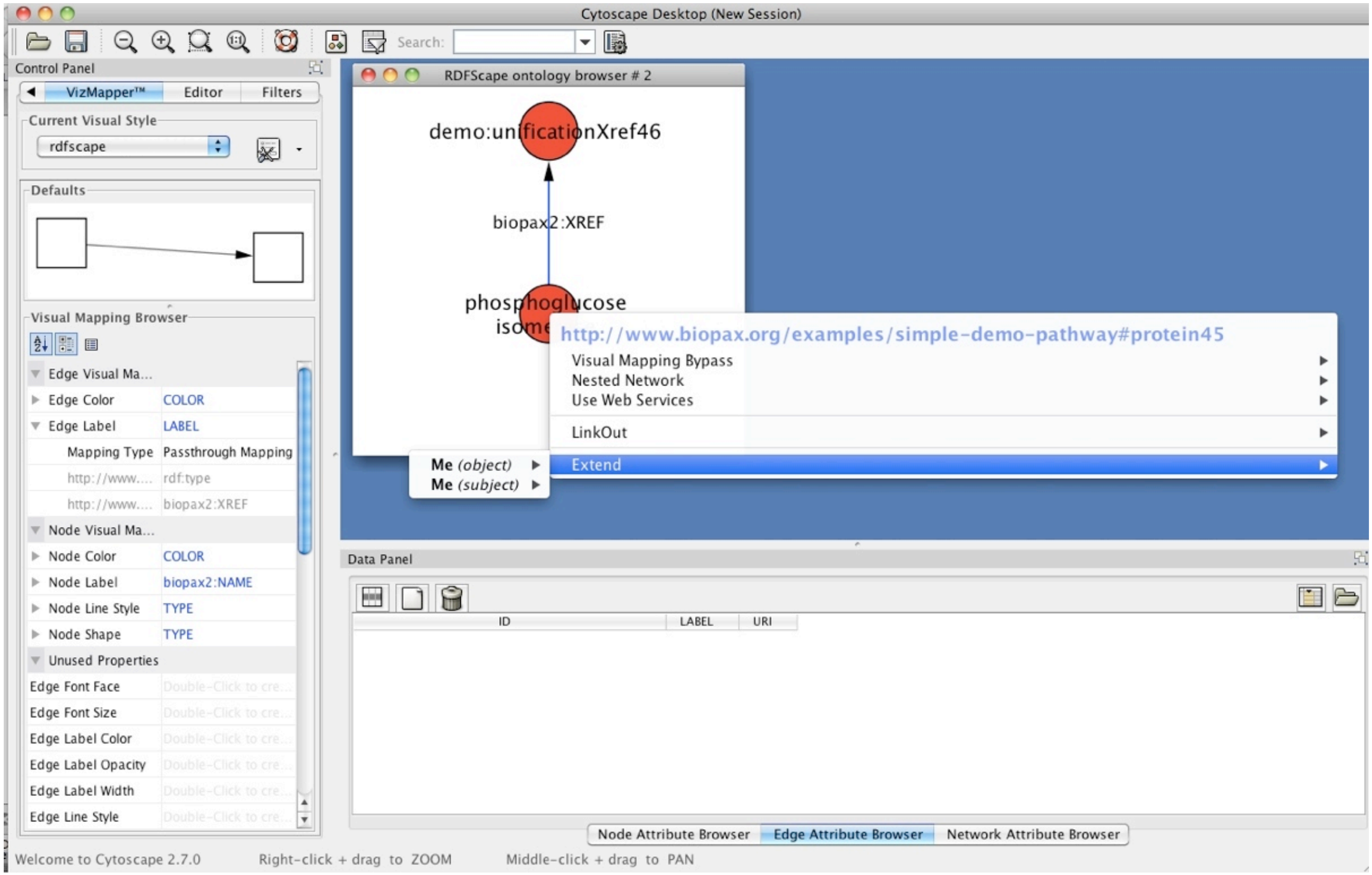
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biopax2:XREF
Node Visual Ma...
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Node Label
biopax2:NAME
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Edge Label Color
Edge Label Opacity
Edge Label Width
Edge Line Style
RDFScape ontology browser # 2
demo:unificationXref46
biopax2:XREF
phosphoglucose
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http://www.biopax.org/examples/simple-demo-pathway#protein45
Visual Mapping Bypass
Nested Network
Use Web Services
LinkOut
Me (object)
Me (subject)
Extend
Data Panel
ID
LABEL
URI
Node Attribute Browser
Edge Attribute Browser
Network Attribute Browser
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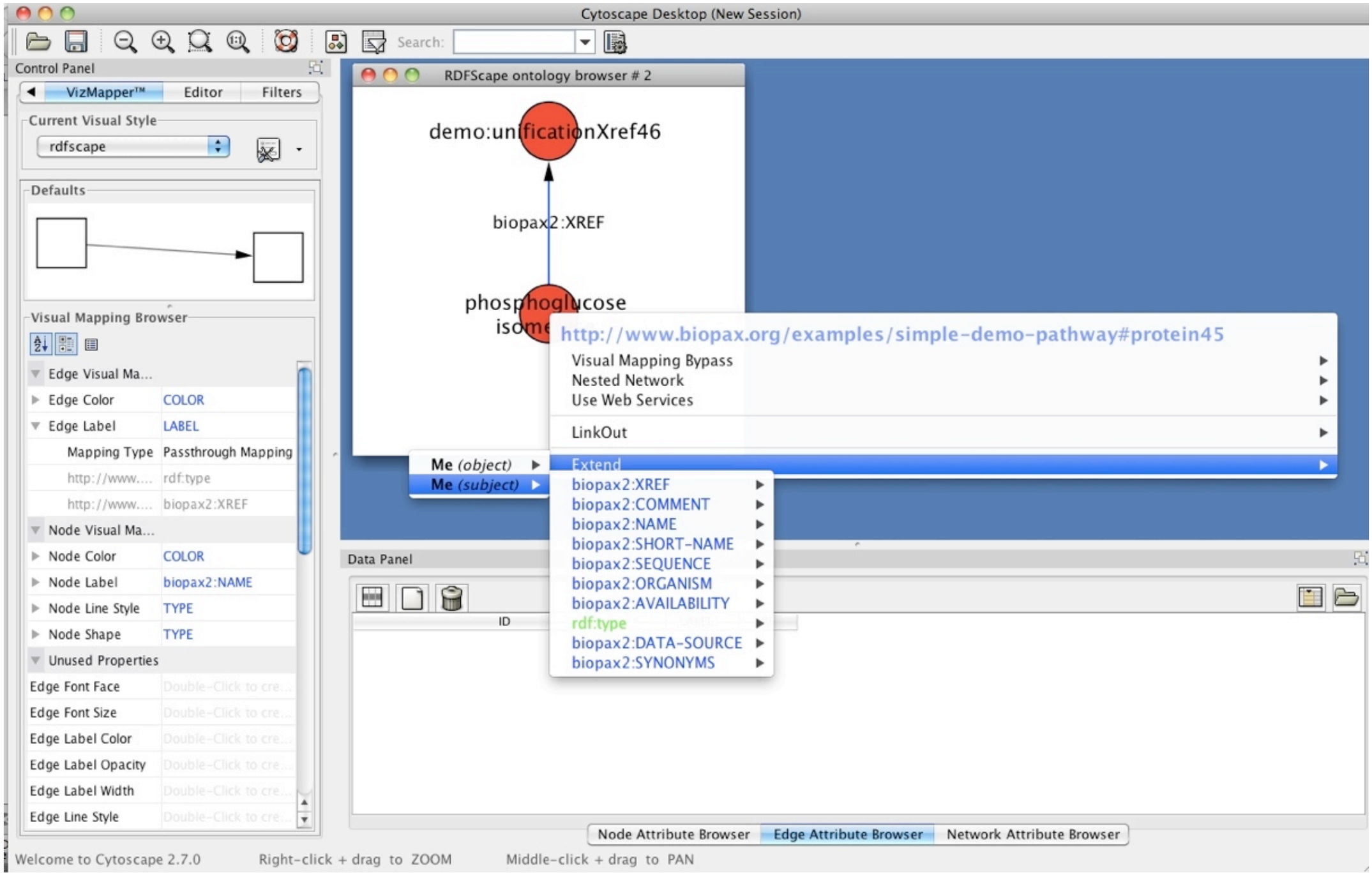
Cytoscape Desktop (New Session)
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Passthrough Mapping
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biopax2:NAME
Node Line Style
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Node Shape
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Edge Font Face
Edge Font Size
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Edge Label Opacity
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Edge Line Style
RDFScape ontology browser # 2
demo:unificationXref46
biopax2:XREF
phosphoglucose
isome
http://www.biopax.org/examples/simple-demo-pathway#protein45
Visual Mapping Bypass
Nested Network
Use Web Services
LinkOut
Me (object)
Me (subject)
Extend
biopax2:XREF
biopax2:COMMENT
biopax2:NAME
biopax2:SHORT-NAME
biopax2:SEQUENCE
biopax2:ORGANISM
biopax2:AVAILABILITY
rdf:type
biopax2:DATA-SOURCE
biopax2:SYNONYMS
Data Panel
ID
Node Attribute Browser
Edge Attribute Browser
Network Attribute Browser
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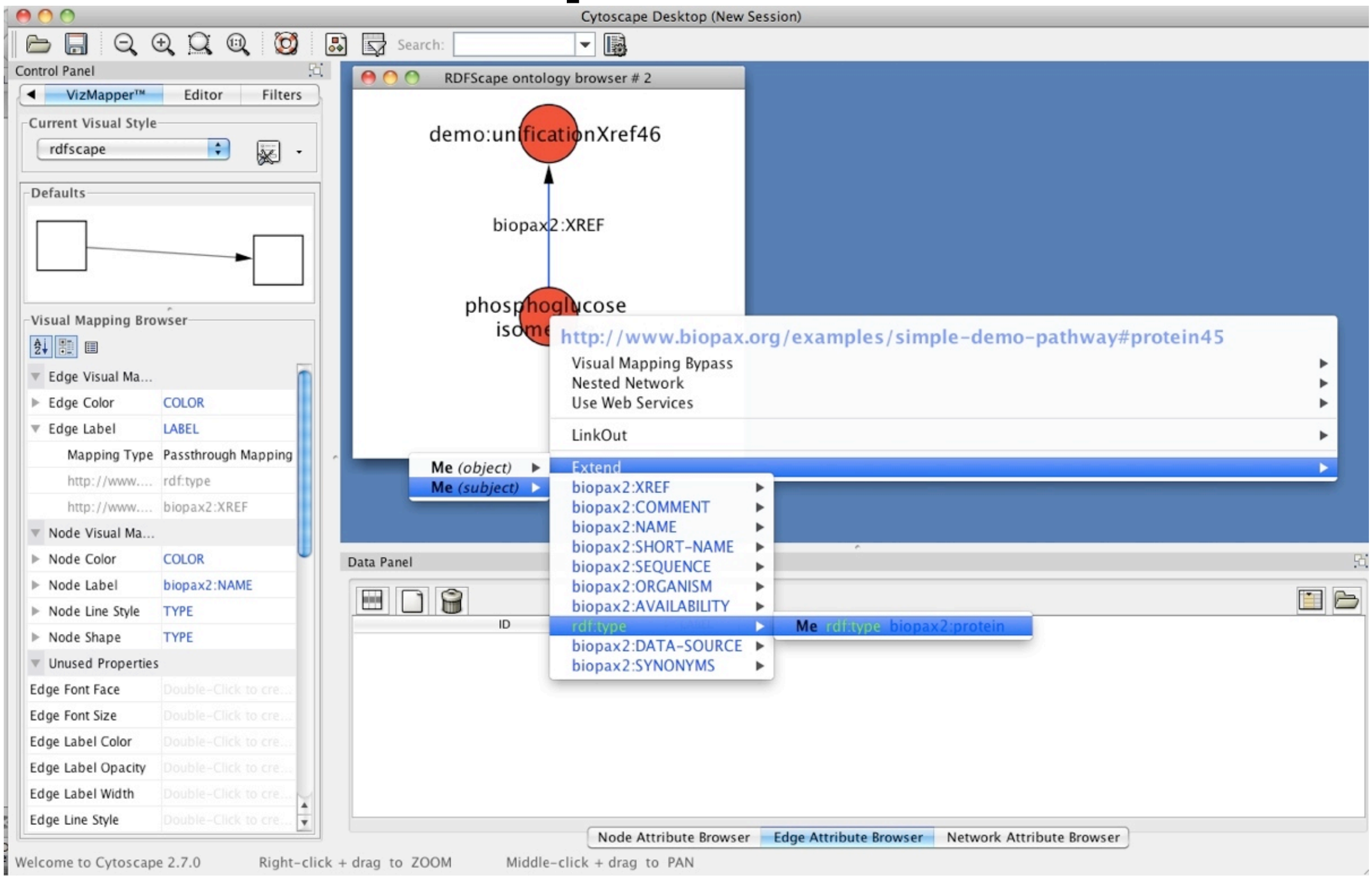
Cytoscape Desktop (New Session)
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Mapping Type
Passthrough Mapping
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biopax2:XREF
Node Visual Ma...
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RDFScape ontology browser # 2
demo:unificationXref46
biopax2:XREF
phosphoglucose
isome
http://www.biopax.org/examples/simple-demo-pathway#protein45
Visual Mapping Bypass
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Me (object)
Me (subject)
Extend
biopax2:XREF
biopax2:COMMENT
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biopax2:SEQUENCE
biopax2:ORGANISM
biopax2:AVAILABILITY
rdf:type
biopax2:DATA-SOURCE
biopax2:SYNONYMS
Me rdf:type biopax2:protein
Data Panel
ID
Node Attribute Browser
Edge Attribute Browser
Network Attribute Browser
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Middle-click + drag to PAN


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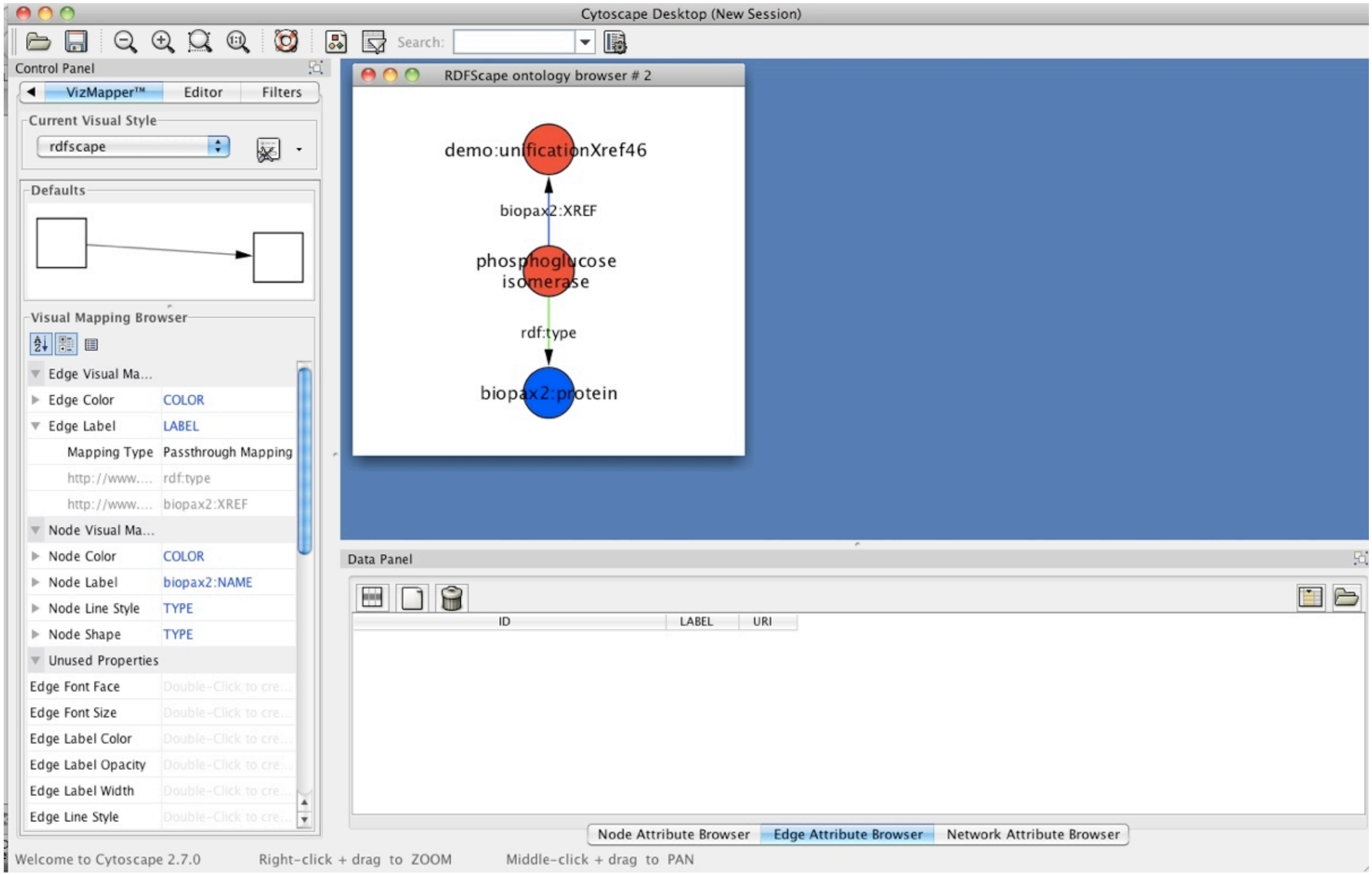
Cytoscape Desktop (New Session)
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Control Panel
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Filters
Current Visual Style
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Defaults
Visual Mapping Browser
Edge Visual Ma...
Edge Color
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Edge 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
Edge Font Size
Edge Label Color
Edge Label Opacity
Edge Label Width
Edge Line Style
RDFScape ontology browser # 2
demo:unificationXref46
biopax2:XREF
phosphoglucose isomerase
rdf:type
biopax2:protein
Data Panel
ID
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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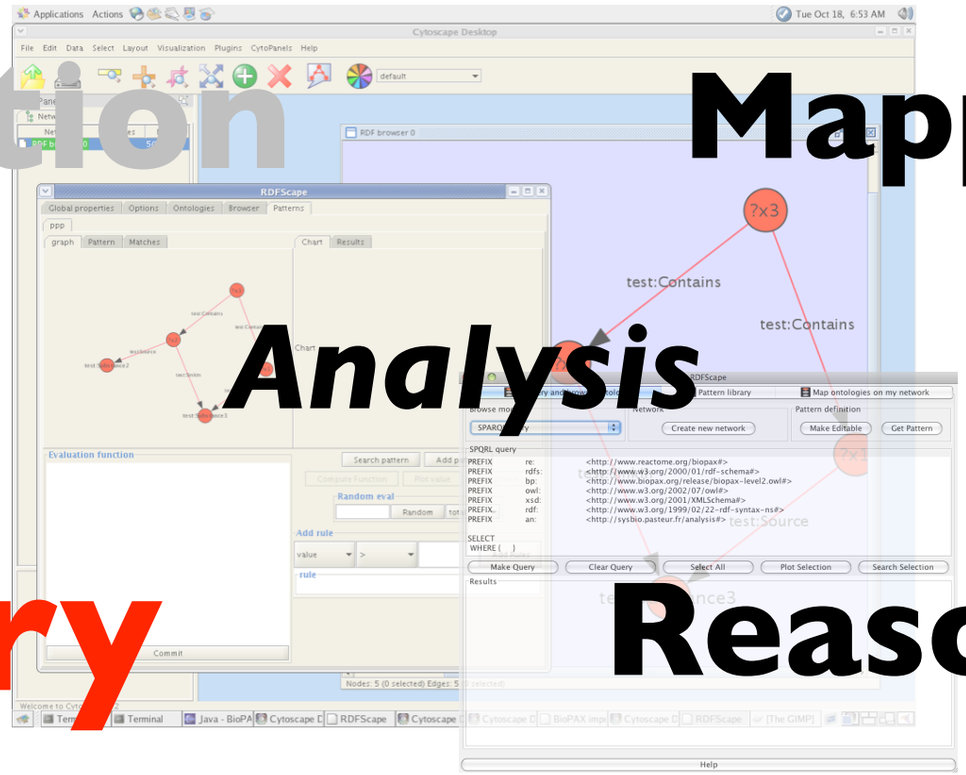
RDFScape = Interface

Inspection

Mapping

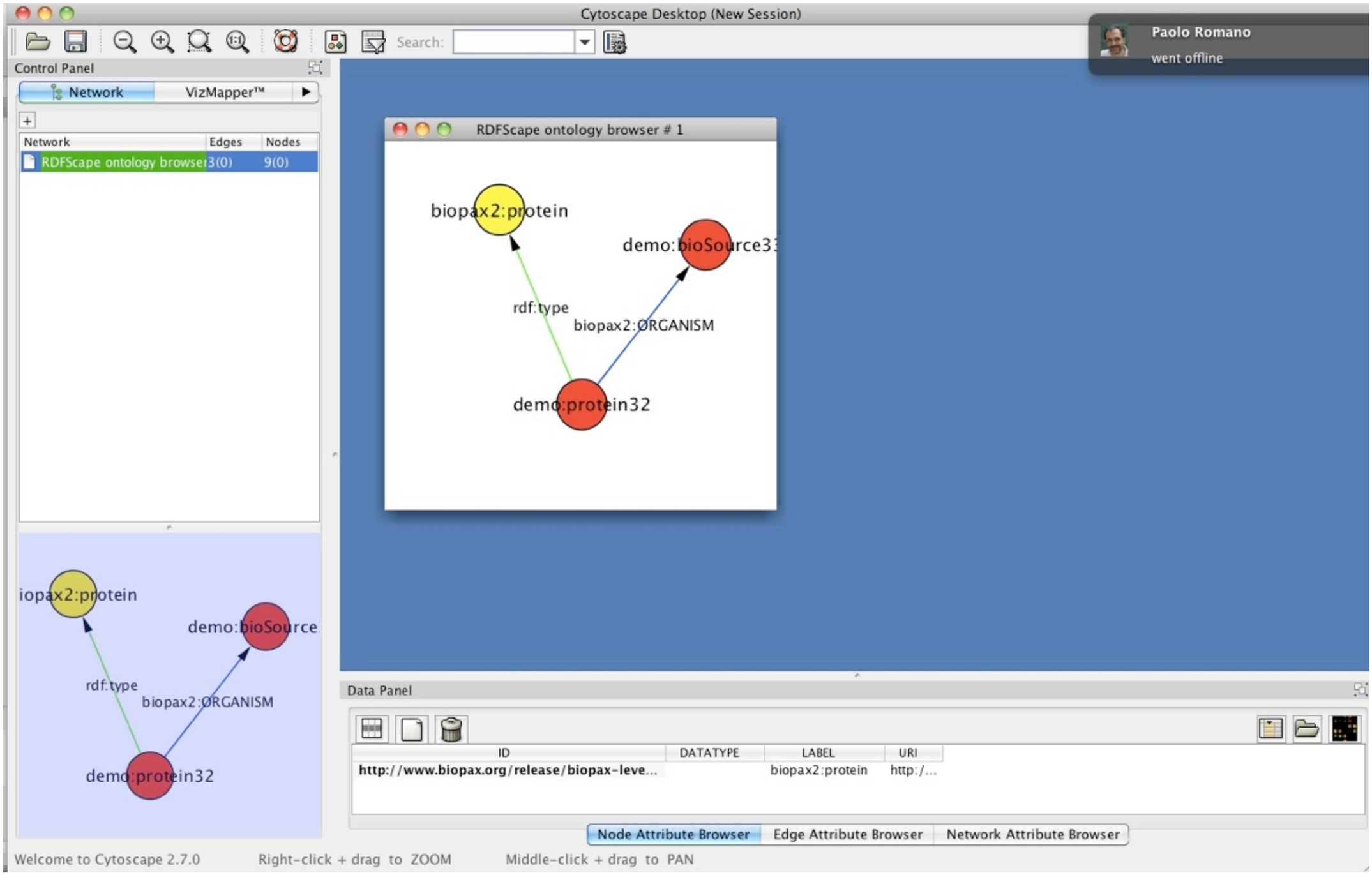


Analysis

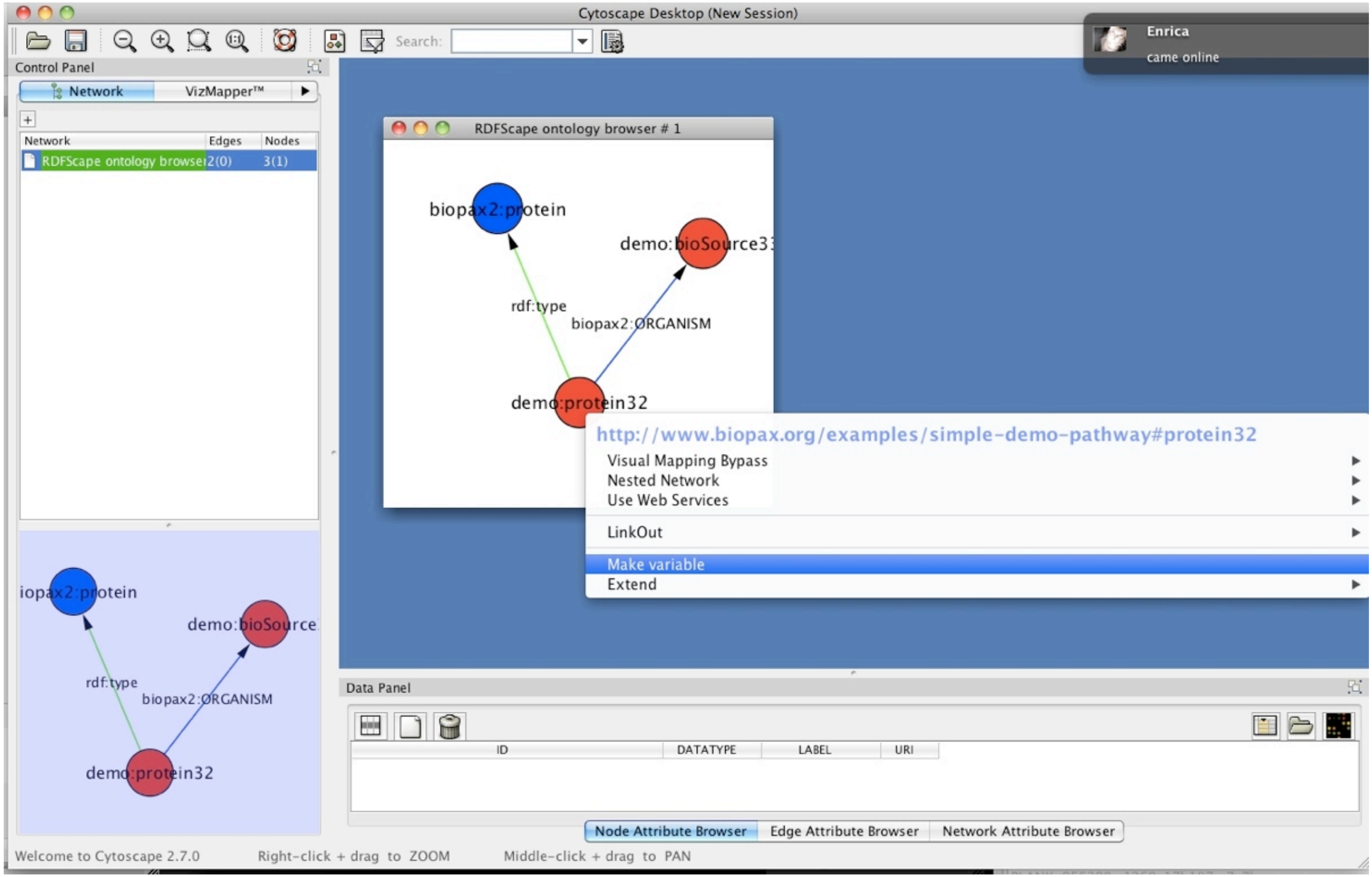
Query

Reasoning

Query


Cytoscape Desktop (New Session)
Search:
Paolo Romano
went offline
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
3(0)
9(0)
RDFScape ontology browser # 1
biopax2:protein
demo:bioSource33
rdf:type
biopax2:ORGANISM
demo:protein32
iopax2:protein
demo:bioSource
rdf:type
biopax2:ORGANISM
demo:protein32
Data Panel
ID
DATATYPE
LABEL
URI
http://www.biopax.org/release/biopax-leve...
biopax2:protein
http:/...
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

Query


Cytoscape Desktop (New Session)
Search:
Enrica
came online
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
2(0)
3(1)
RDFScape ontology browser # 1
biopax2:protein
demo:bioSource33
rdf:type
biopax2:ORGANISM
demo:protein32
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
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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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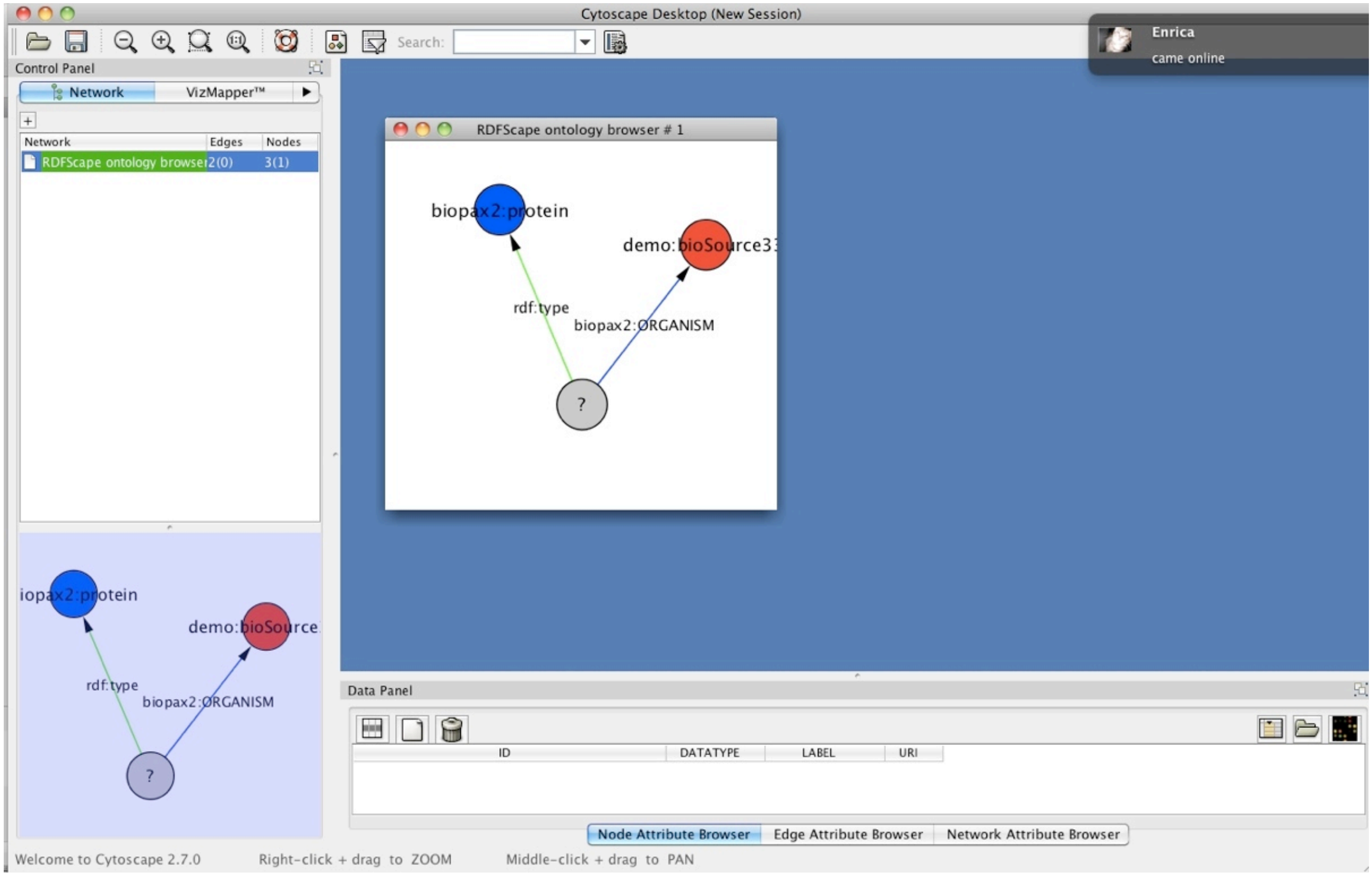
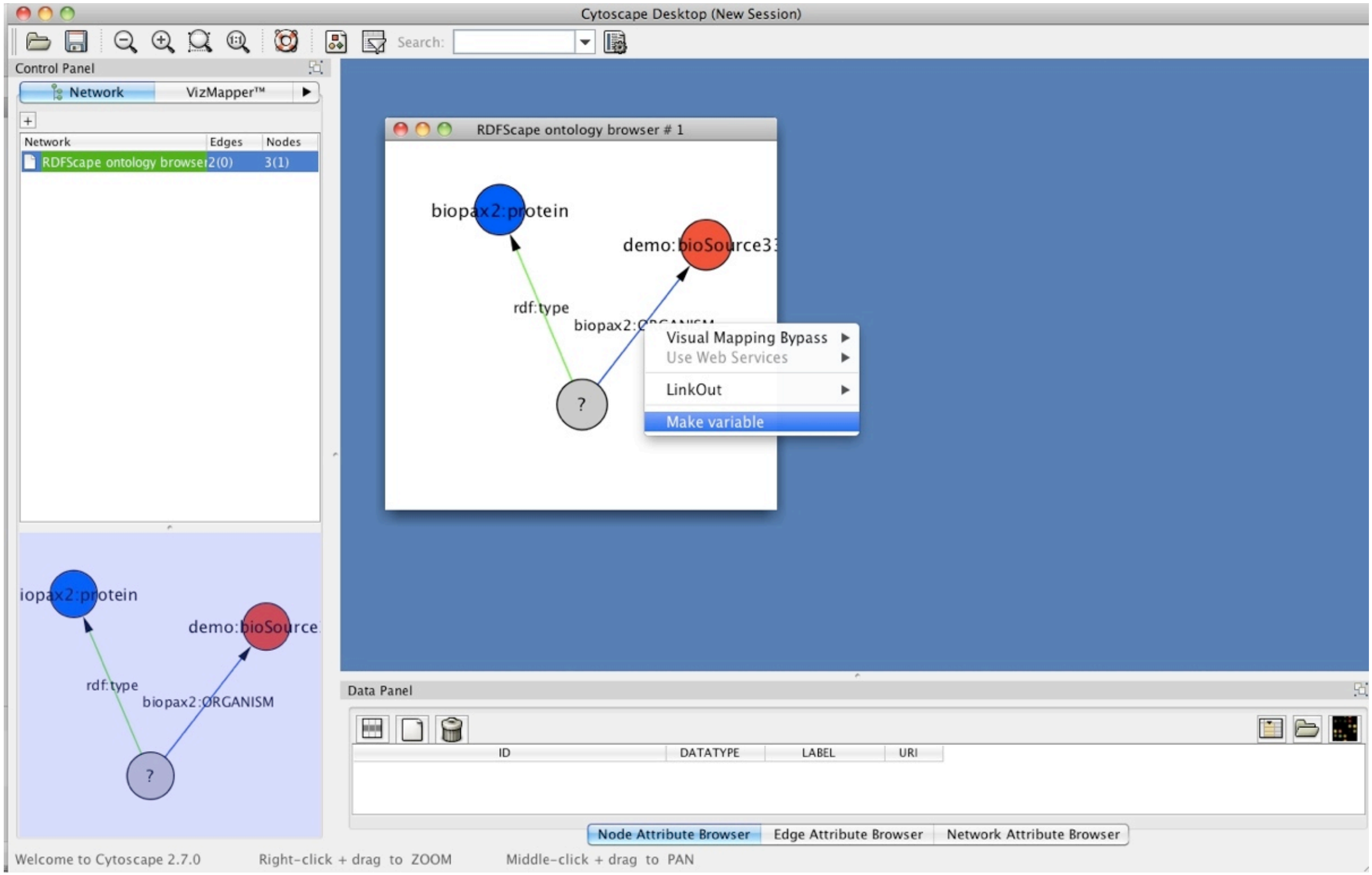
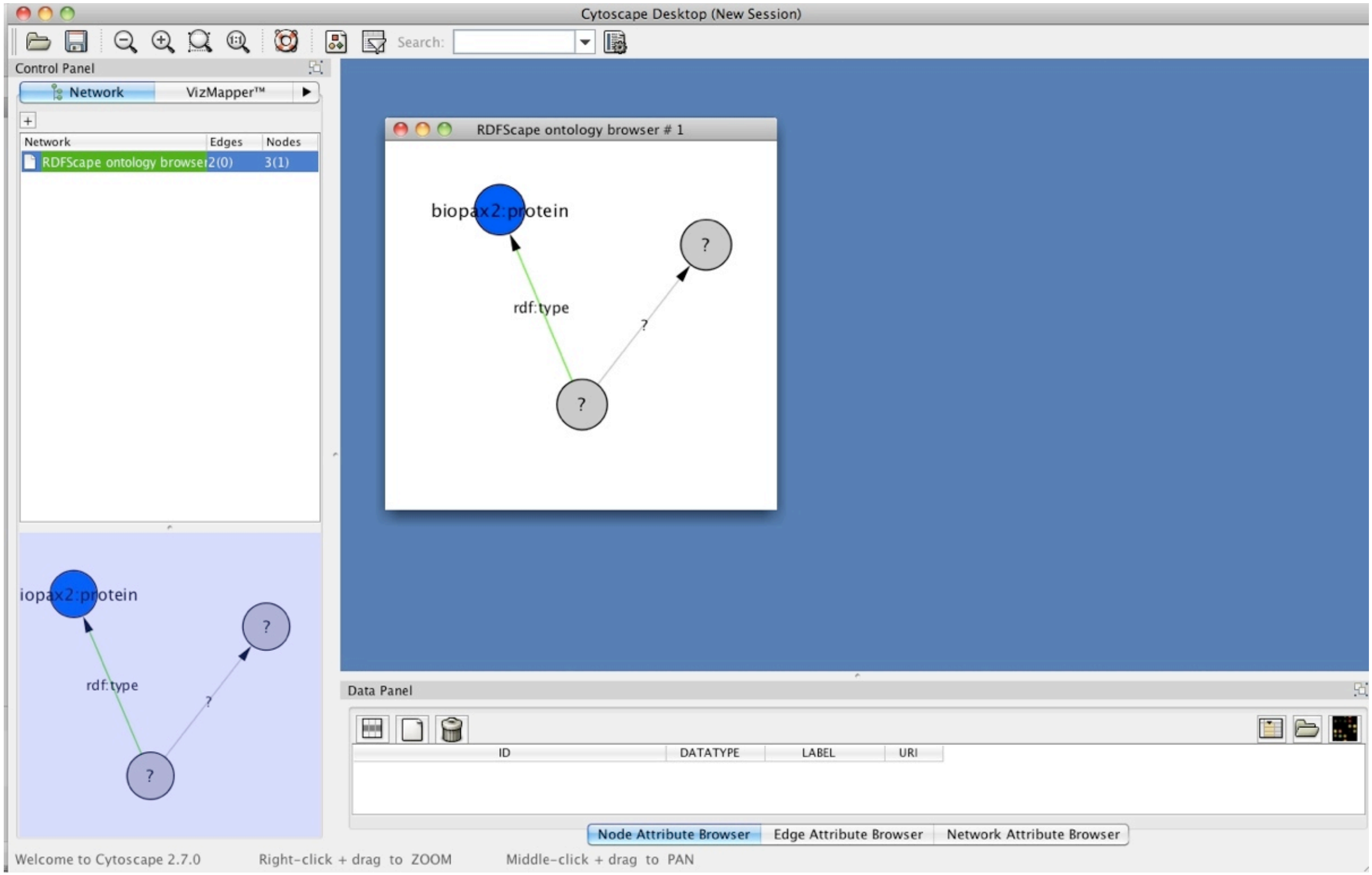
Query


Cytoscape Desktop (New Session)
Search:
Enrica
came online
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
2(0)
3(1)
RDFScape ontology browser # 1
biopax2:protein
demo:bioSource3
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

Query


Cytoscape Desktop (New Session)
Search:
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
2(0)
3(1)
RDFScape ontology browser # 1
biopax2:protein
demo:bioSource3
rdf:type
biopax2:ORGANISM
?
Visual Mapping Bypass
Use Web Services
LinkOut
Make variable
iopax2: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

Query


Cytoscape Desktop (New Session)
Search:
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
2(0)
3(1)
RDFScape ontology browser # 1
biopax2:protein
rdf:type
?
?
?
Data Panel
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LABEL
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Node Attribute Browser
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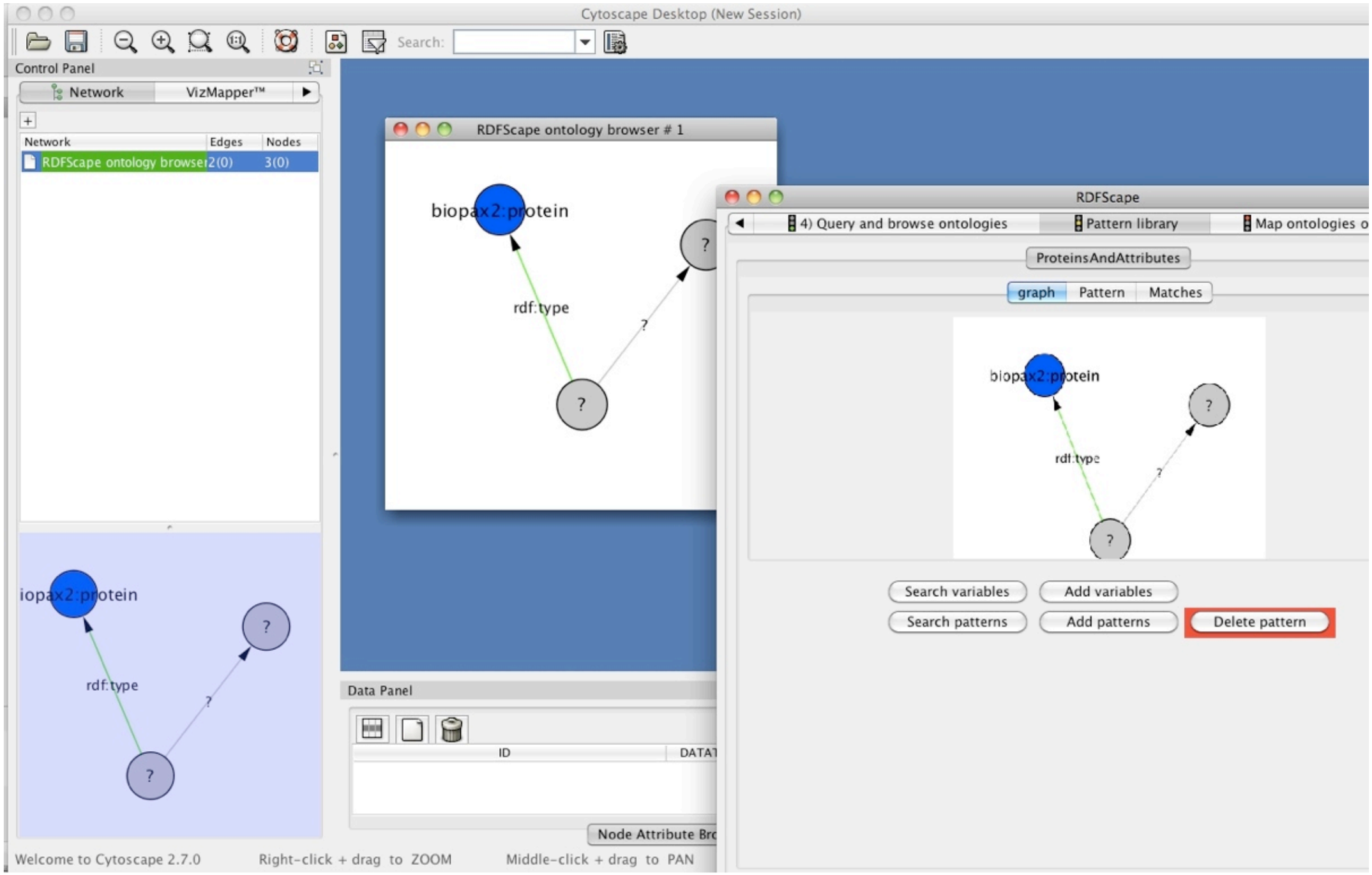
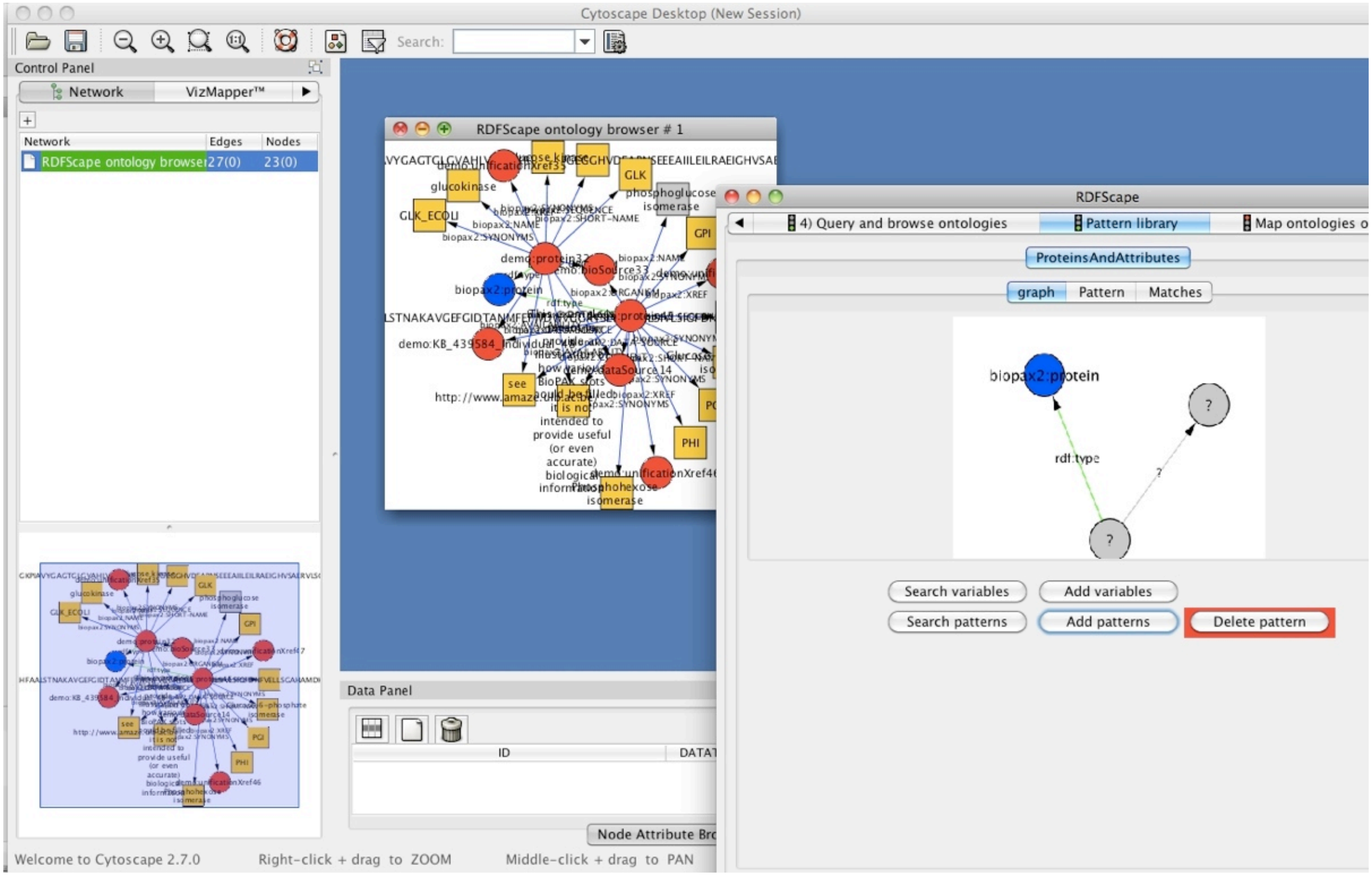
Welcome to Cytoscape 2.7.0
Right-click + drag to ZOOM
Middle-click + drag to PAN

Query


Cytoscape Desktop (New Session)
Search:
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
2(0)
3(0)
RDFScape ontology browser # 1
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
Node Attribute Bro
Welcome to Cytoscape 2.7.0
Right-click + drag to ZOOM
Middle-click + drag to PAN

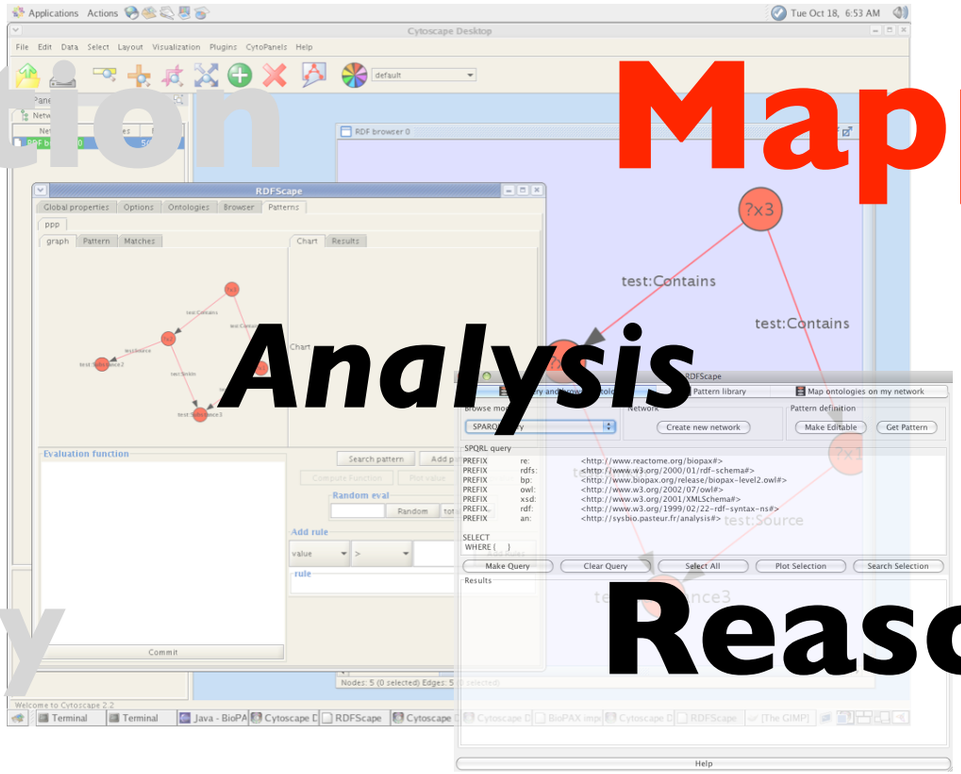
Query


Cytoscape Desktop (New Session)
Search:
Control Panel
Network
VizMapper™
Network
Edges
Nodes
RDFScape ontology browser
27(0)
23(0)
RDFScape ontology browser # 1
RDFScape
4) Query and browse ontologies
Pattern library
ProteinsAndAttributes
graph
Pattern
Matches
biopax2:protein
rdf:type
Search variables
Add variables
Search patterns
Add patterns
Delete pattern
Data Panel
ID
Node Attribute Br
Welcome to Cytoscape 2.7.0
Right-click + drag to ZOOM
Middle-click + drag to PAN

RDFScape = Interface

Inspection

Mapping

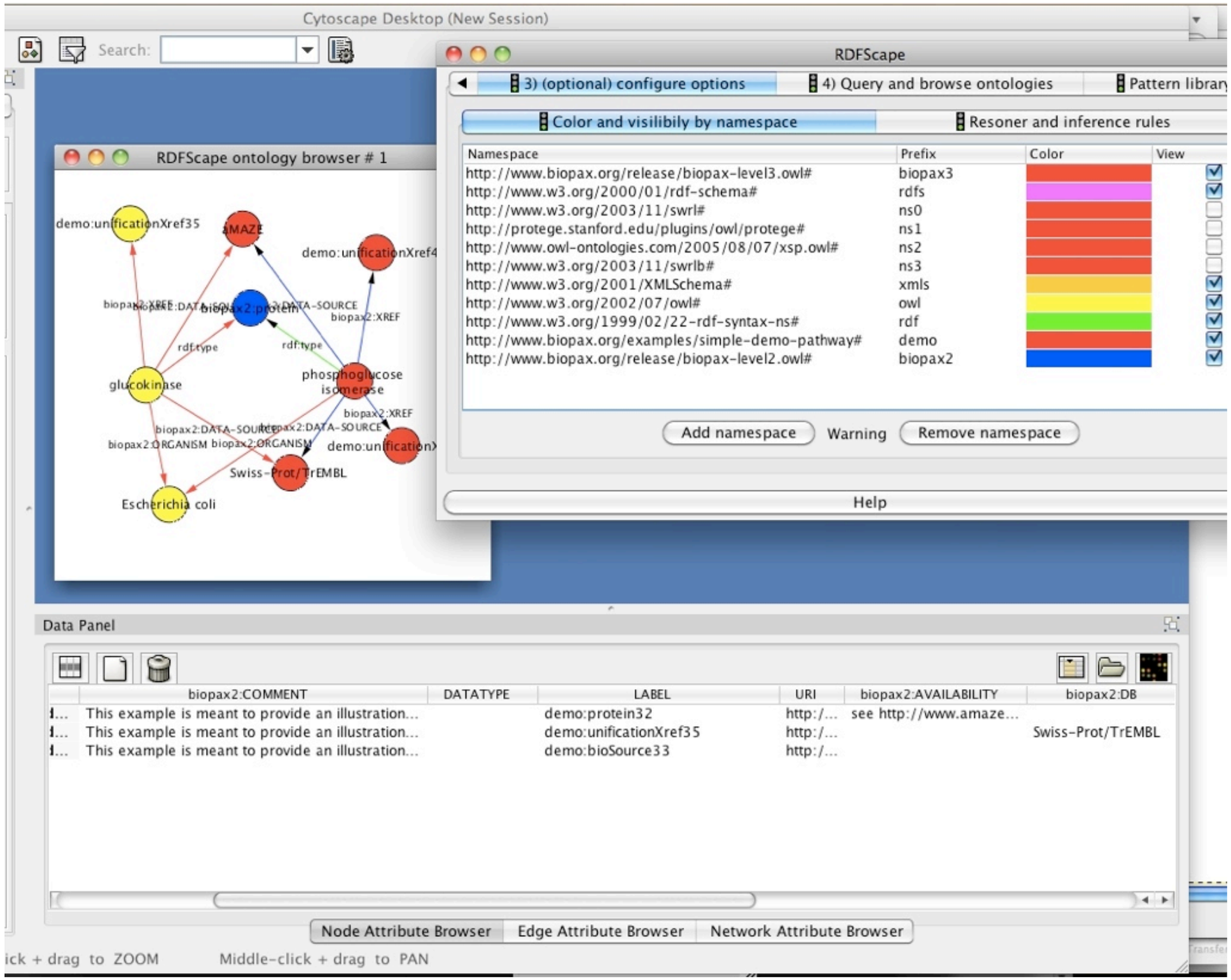


Analysis

Query

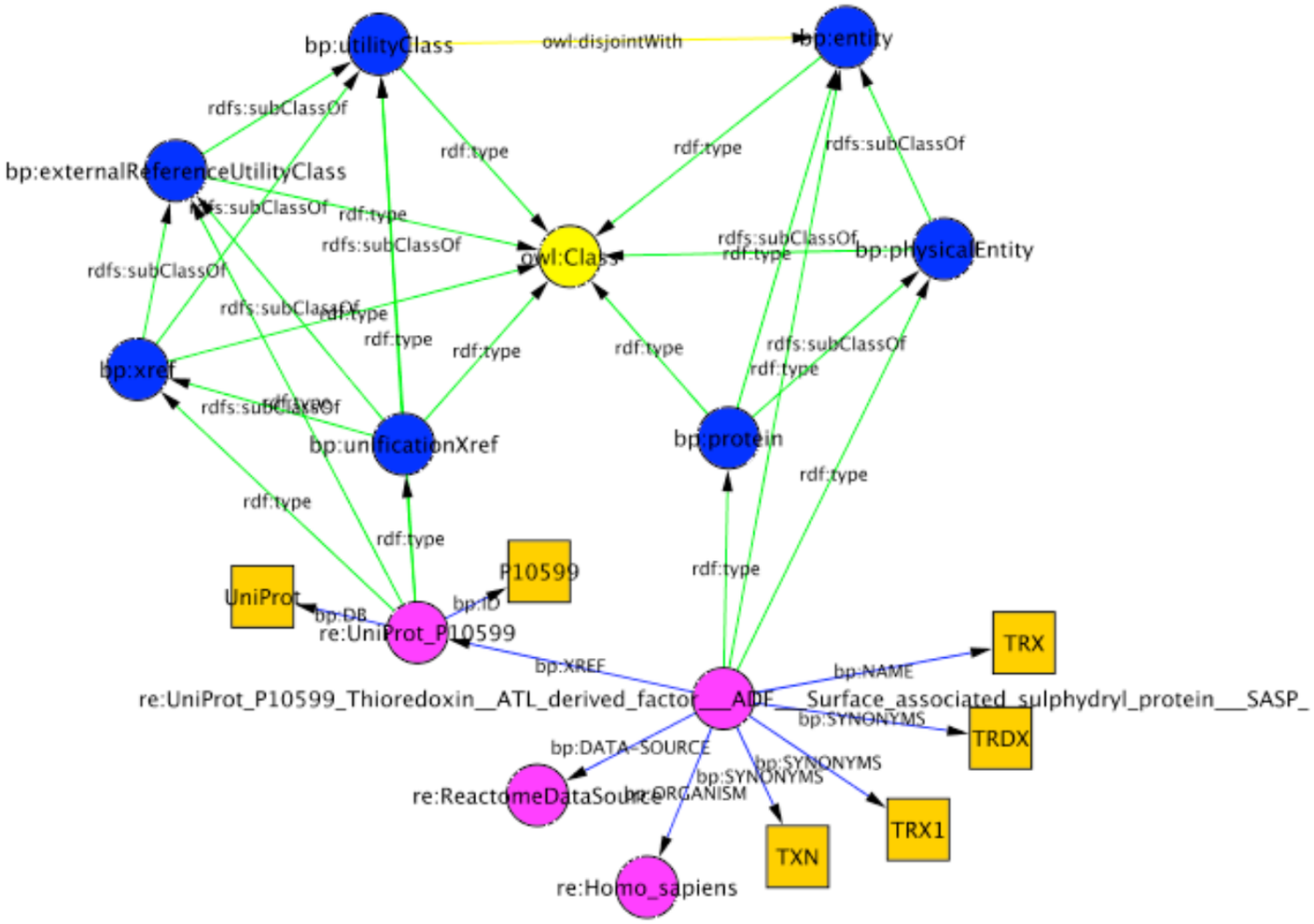
Reasoning

Mapping



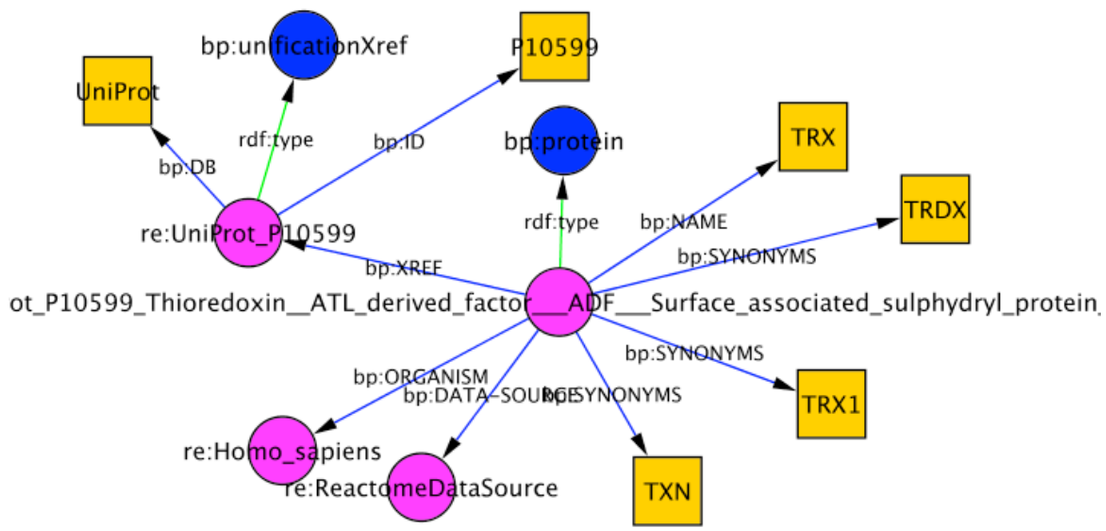
- selection/ colouring by namespace
- datatype properties as attributes
- URIs represented as multiple nodes

Mapping



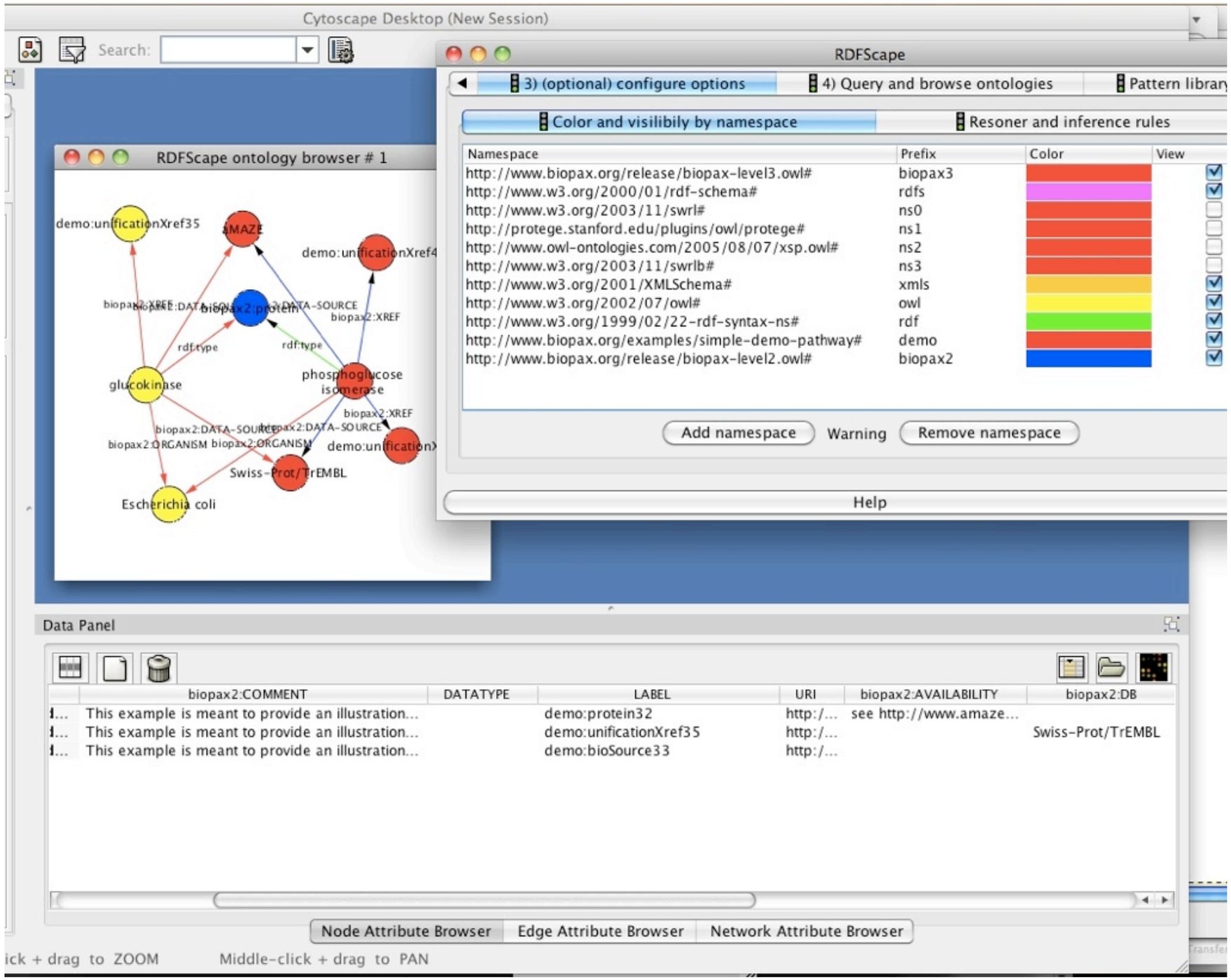
- selection/ colouring by namespace
- datatype properties as attributes
- URIs represented as multiple nodes

Mapping



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

Mapping



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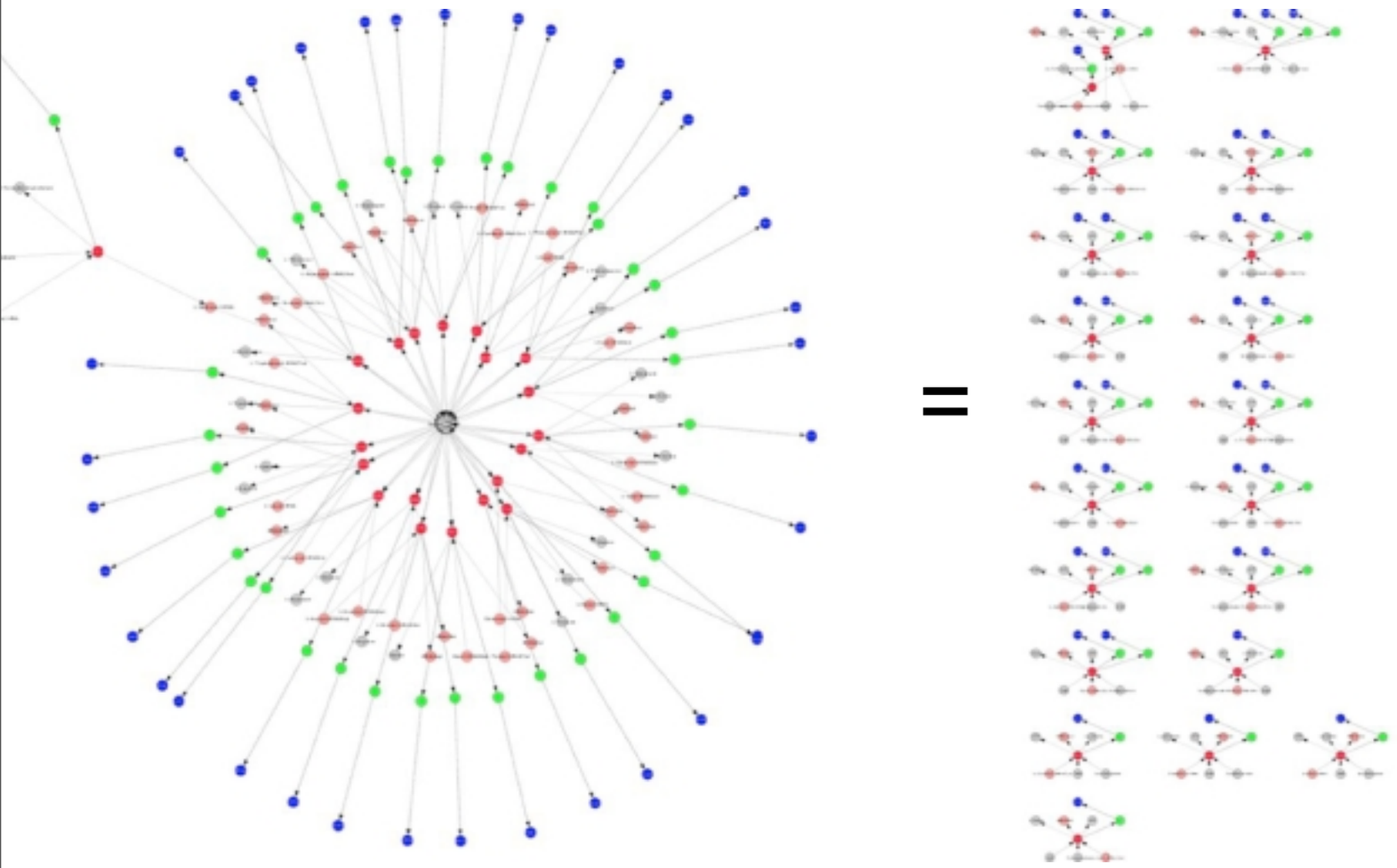
Mapping

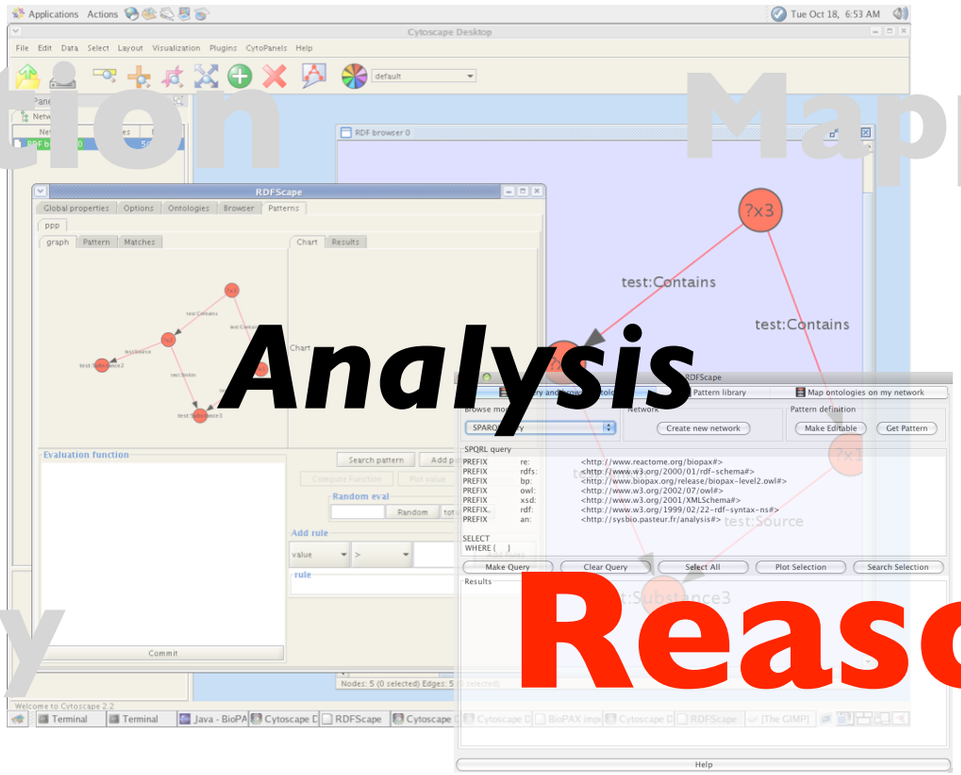


ATP, H2O...

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

RDFScape = Interface

Inspection Mapping

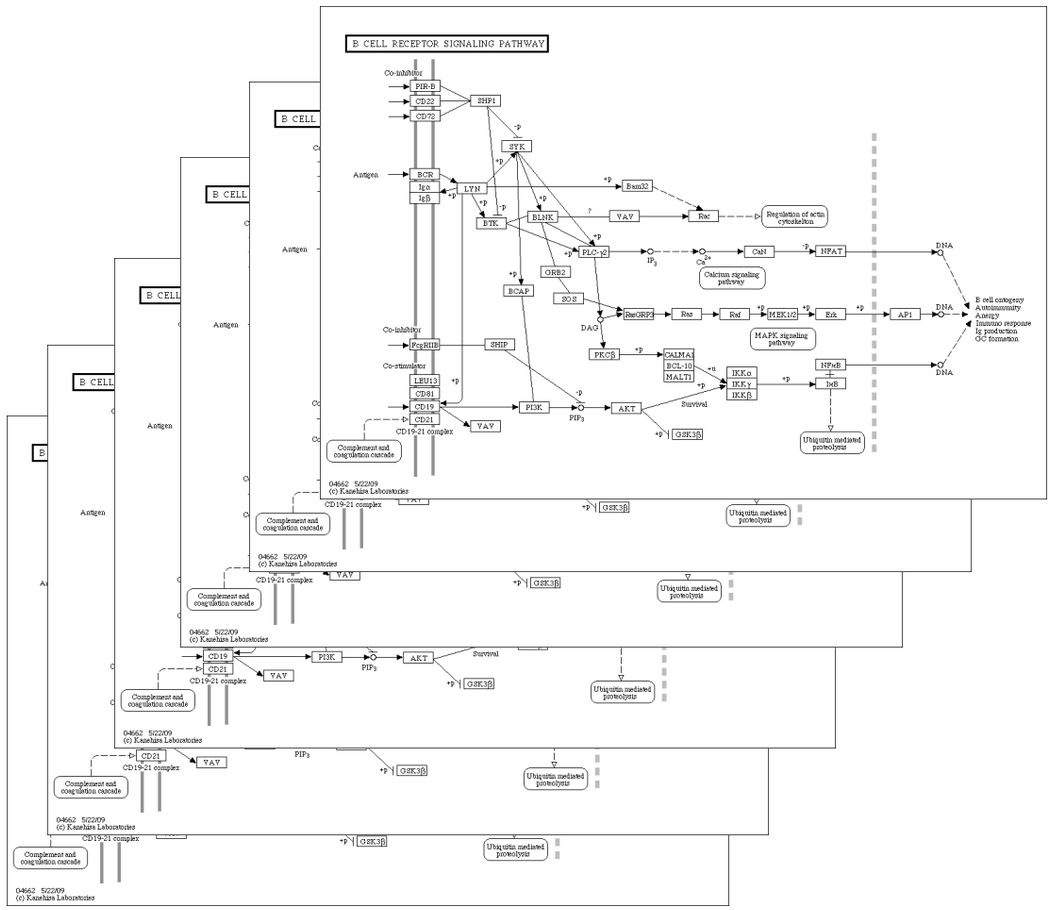


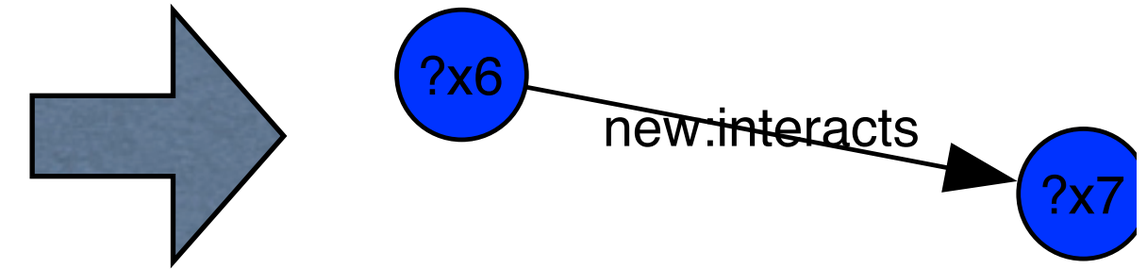
Analysis

Query

Reasoning

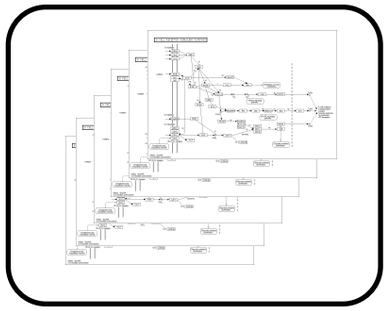
Reasoning


B CELL RECEPTOR SIGNALING PATHWAY
Co-inhibitor
PIR-B
CD22
CD72
SHP1
Antigen
BCR
Ig α
Ig β
LYN
SYK
BTK
BLNK
VAV
Bam32
Rac
Regulation of actin cytoskeleton
PLC-γ2
GRB2
SOS
BCAP
RasGRP3
Ras
Raf
MEK1/2
Erk
AP1
DNA
B cell ontogeny
Autoimmunity
Anergy
Immune response
Ig production
GC formation
MAPK signaling pathway
Calcium signaling pathway
CaM
NFAT
DAG
PKCβ
Co-stimulator
FcgRIIB
SHIP
LEU13
CD81
CD19
CD21
CD19-21 complex
PI3K
PIP3
AKT
Survival
GSK3β
CALMA
BCL-10
MALT1
IKKα
IKKγ
IKKβ
NFκB
IκB
Ubiquitin mediated proteolysis
Complement and coagulation cascade
04662 5/22/09
(c) Kanehisa Laboratories

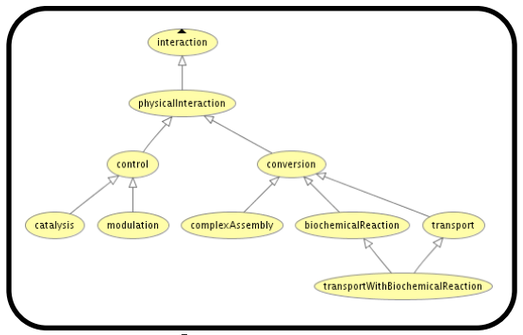

?x6
new:interacts
?x7


Andrea Splendiani, Visualisation and Analysis of Biological Networks on the Web
BioHackathon3 Symposium

Reasoning



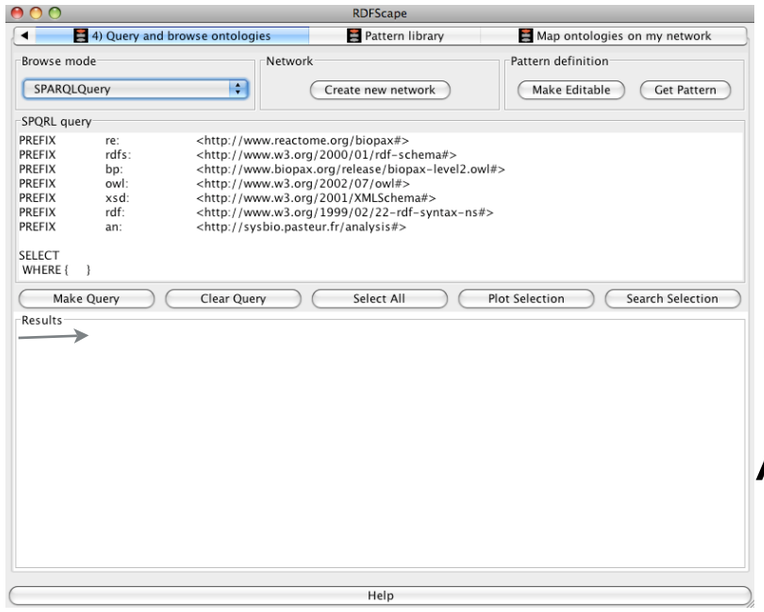
A collection of pathways: biological facts



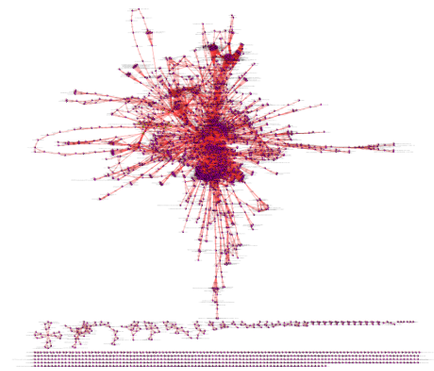
An ontology: a meaning for facts (interpretation)

```
[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:PHYSICAL'ENTITY ?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)



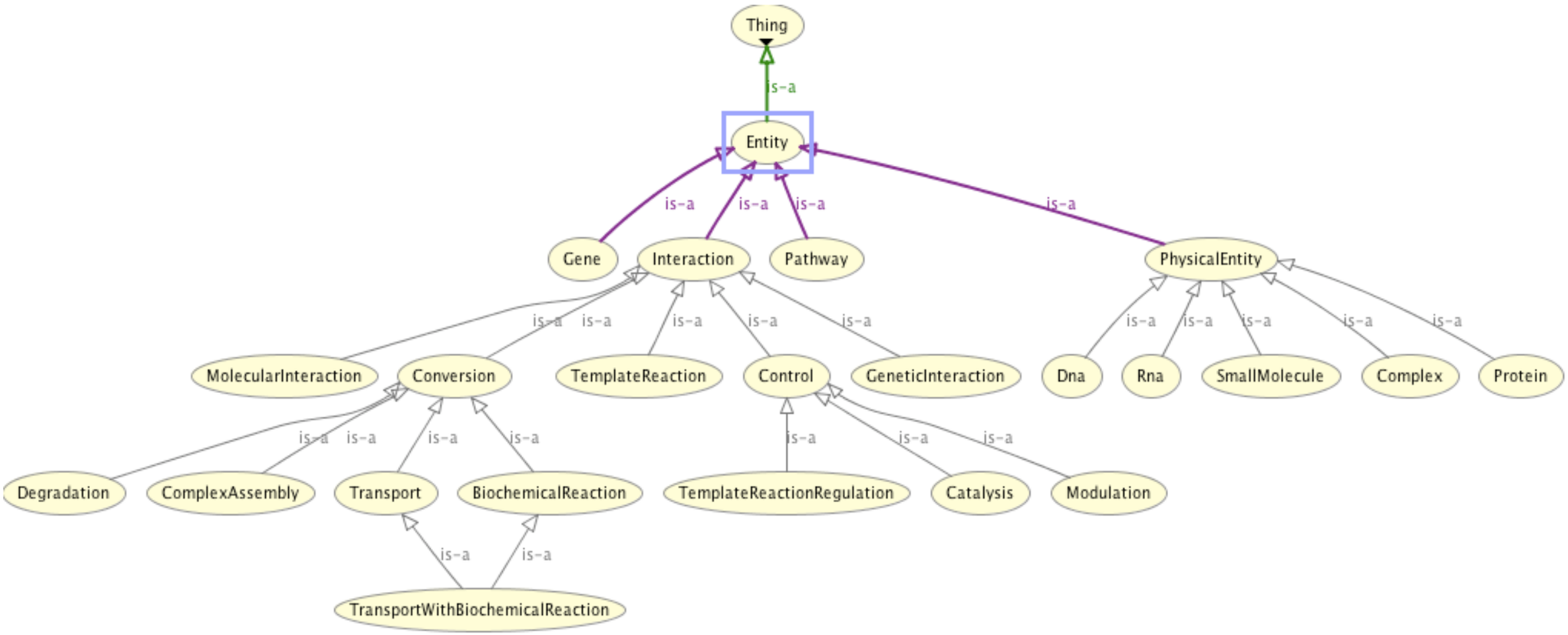
Visualization

Analysis

Abstraction of pathways as interactions

Queries

Reasoning


Thing
is-a
Entity
is-a
is-a
is-a
is-a
Gene
Interaction
Pathway
PhysicalEntity
is-a
is-a
is-a
is-a
is-a
is-a
is-a
is-a
is-a
MolecularInteraction
Conversion
TemplateReaction
Control
GeneticInteraction
Dna
Rna
SmallMolecule
Complex
Protein
is-a
is-a
is-a
is-a
is-a
is-a
is-a
Degradation
ComplexAssembly
Transport
BiochemicalReaction
TemplateReactionRegulation
Catalysis
Modulation
is-a
is-a
TransportWithBiochemicalReaction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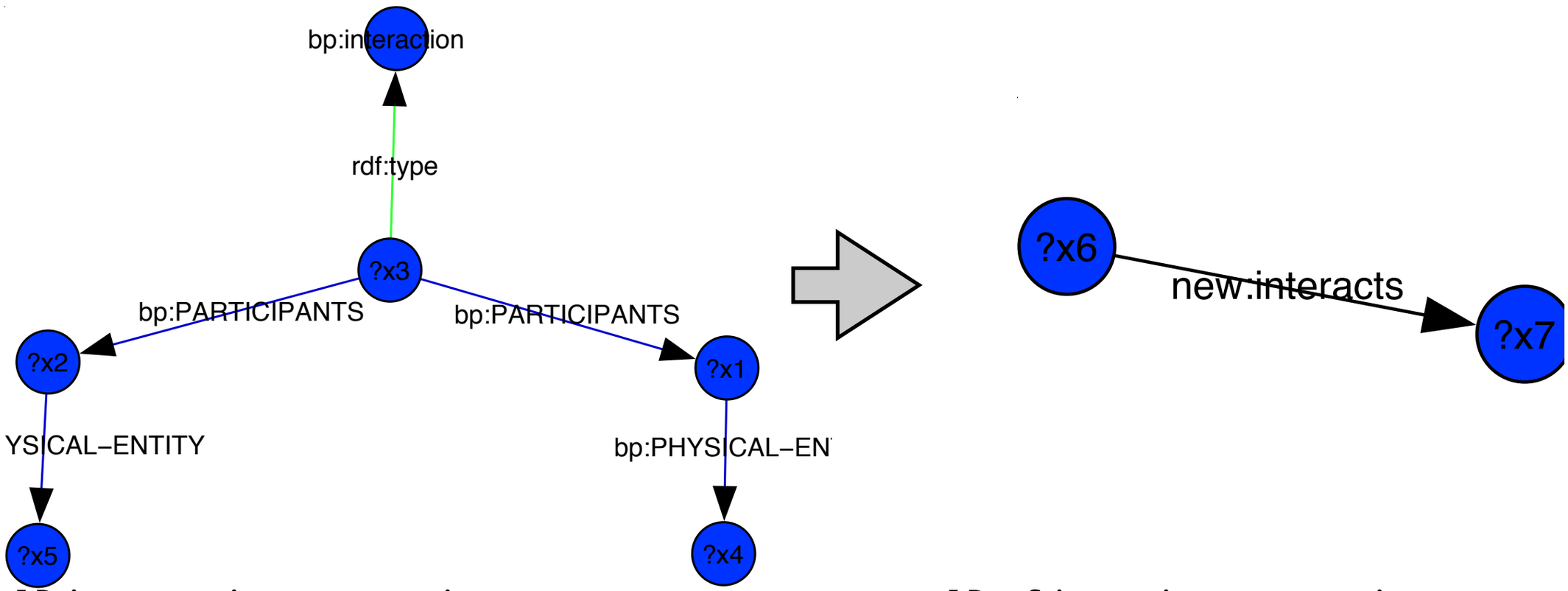
BioHackathon3 Symposium

Reasoning



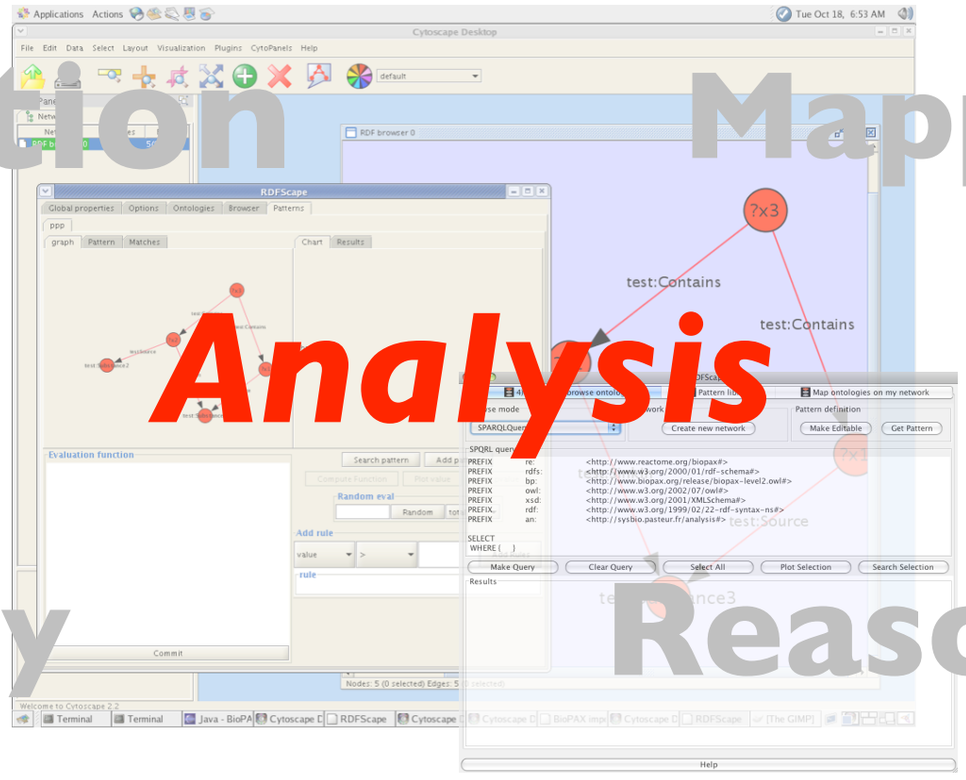

```
[Direct-interaction:
(?interactor new:dirInt ?p)
<-
(?x rdf:type bp:interaction)
(?x bp:PARTICIPANTS ?px)
(?px bp:PHYSICAL-ENTITY ?p)]
```

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

RDFScape = Interface

Inspection

Mapping



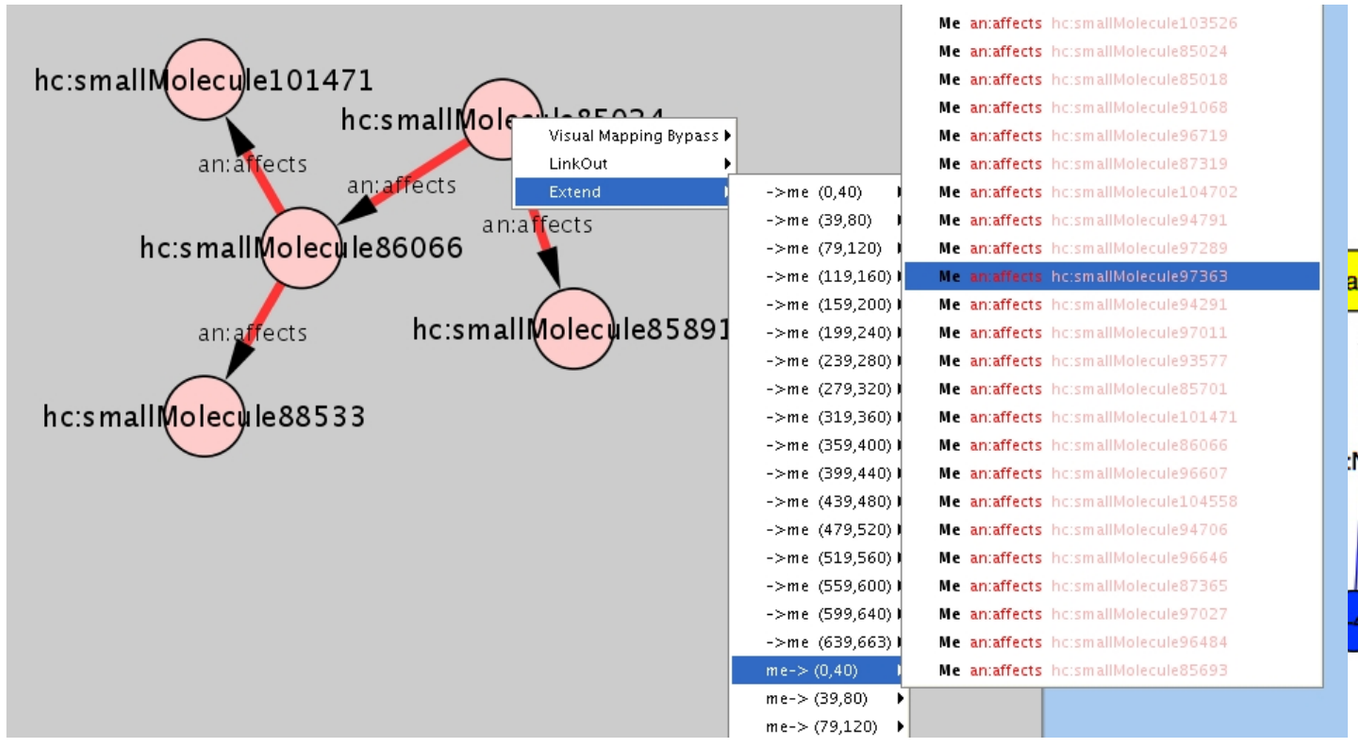
Analysis

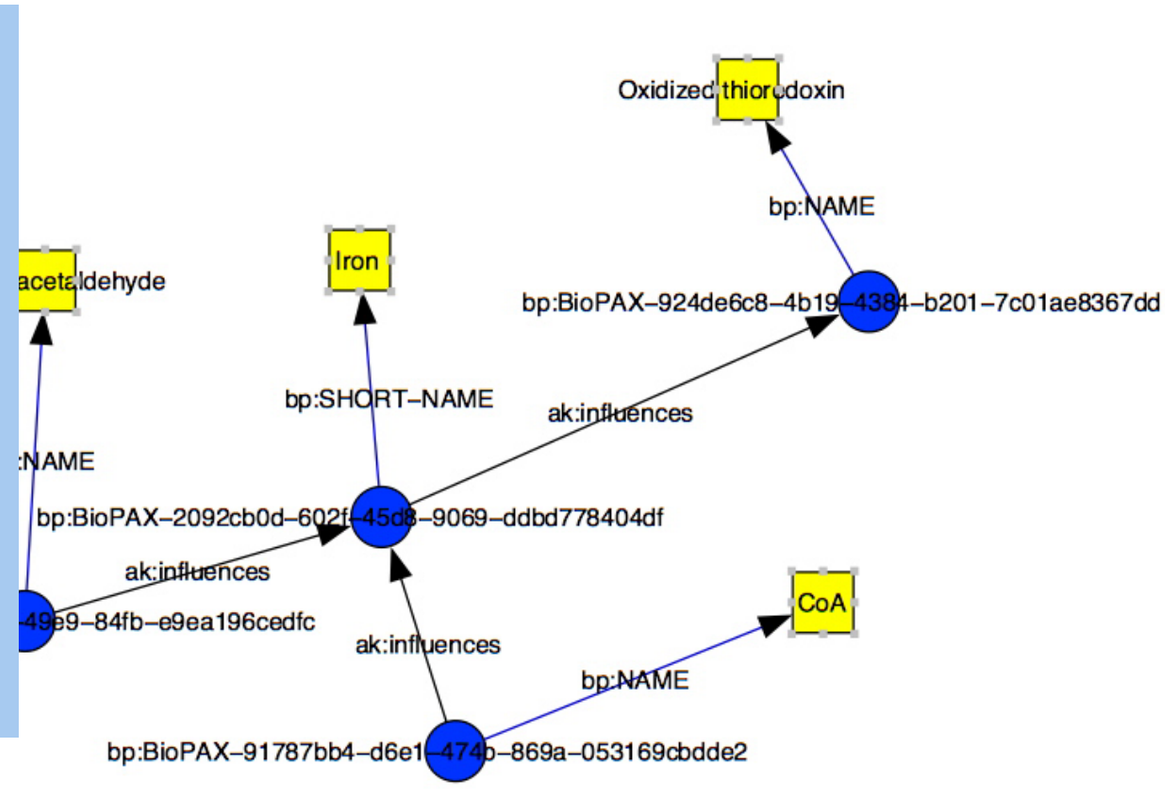
Query

Reasoning

Analysis

(Reasoning on pathways)





View of pathways as an influence graph

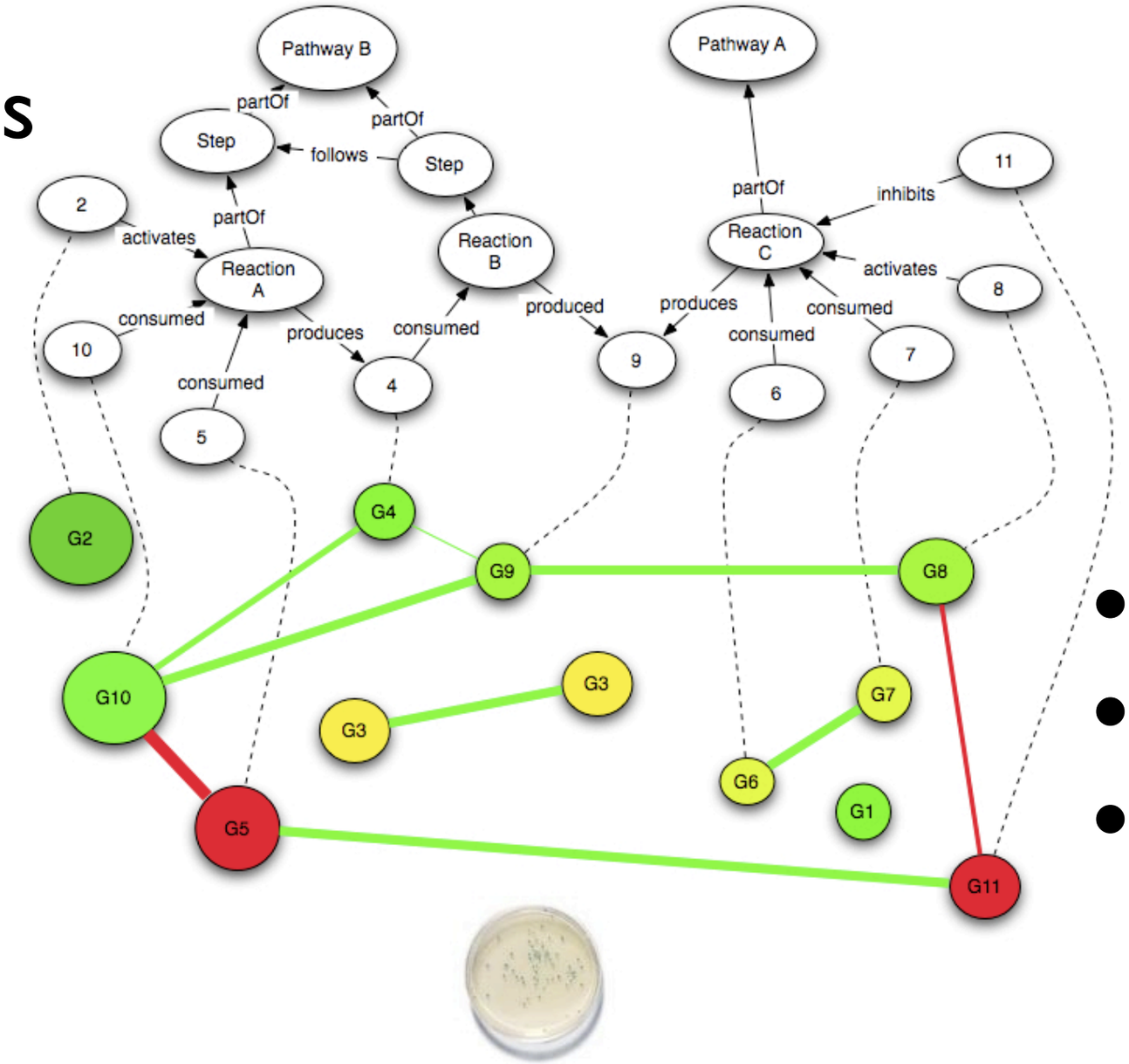
[influence: (?x ak:influences ?y) <- (?p1 rdf:type bp:biochemicalReaction)
(?p2 rdf:type bp:biochemicalReaction)
(?p1 bp:RIGHT ?k1)(?k1 bp:PHYSICAL-ENTITY ?k)
(?p2 bp:LEFT ?k2)(?k2 bp:PHYSICAL-ENTITY ?k)
(?p1 bp:LEFT ?k3)(?k3 bp:PHYSICAL-ENTITY ?x)
(?p2 bp:RIGHT ?k4)(?k4 bp:PHYSICAL-ENTITY ?y)]

inference rules:
definition of "influence"

Analysis

(Ontologies and data)

- Ontologies
- General
- A-priori

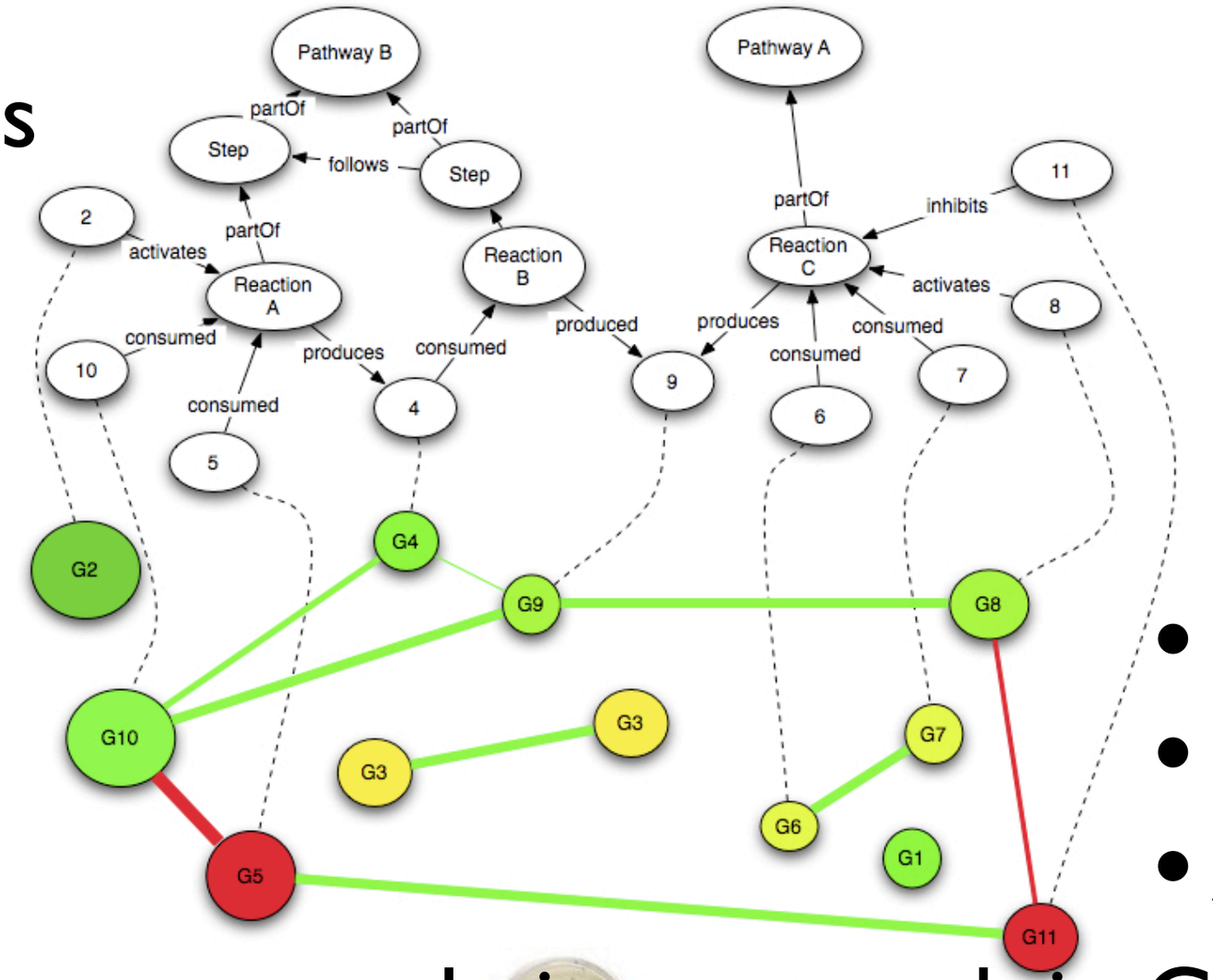


- Data
- Specific
- A-posteriori

Analysis

(Ontologies and data)

- Ontologies
- General
- A-priori

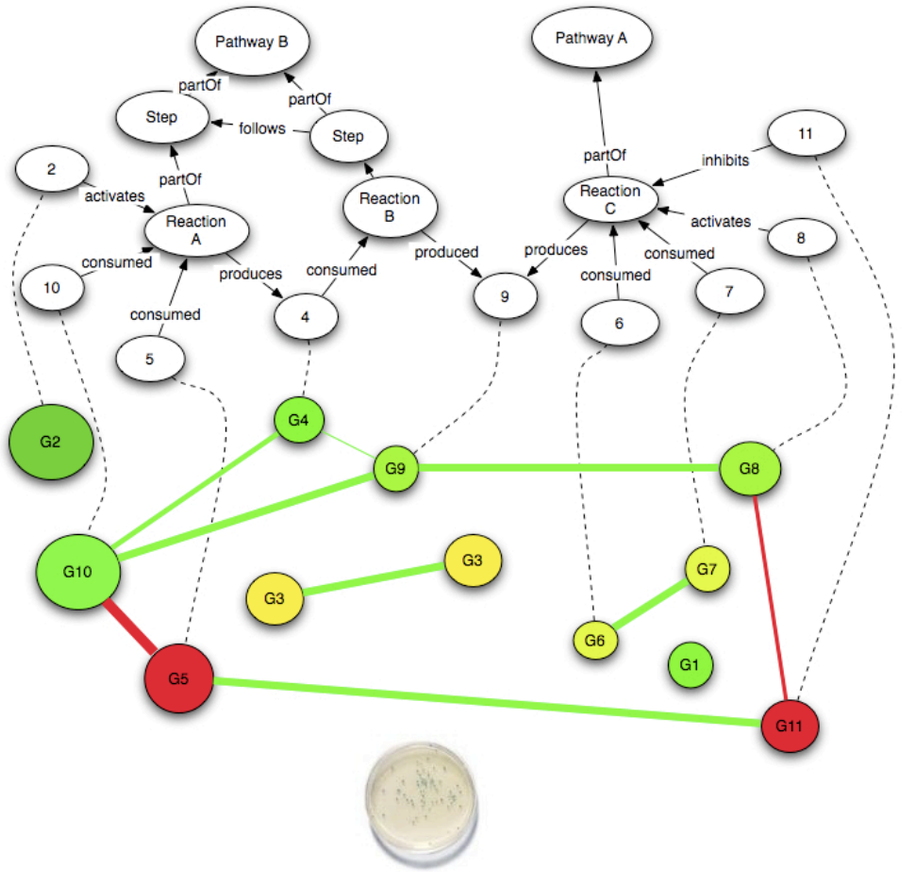


- Data
- Specific
- A-posteriori

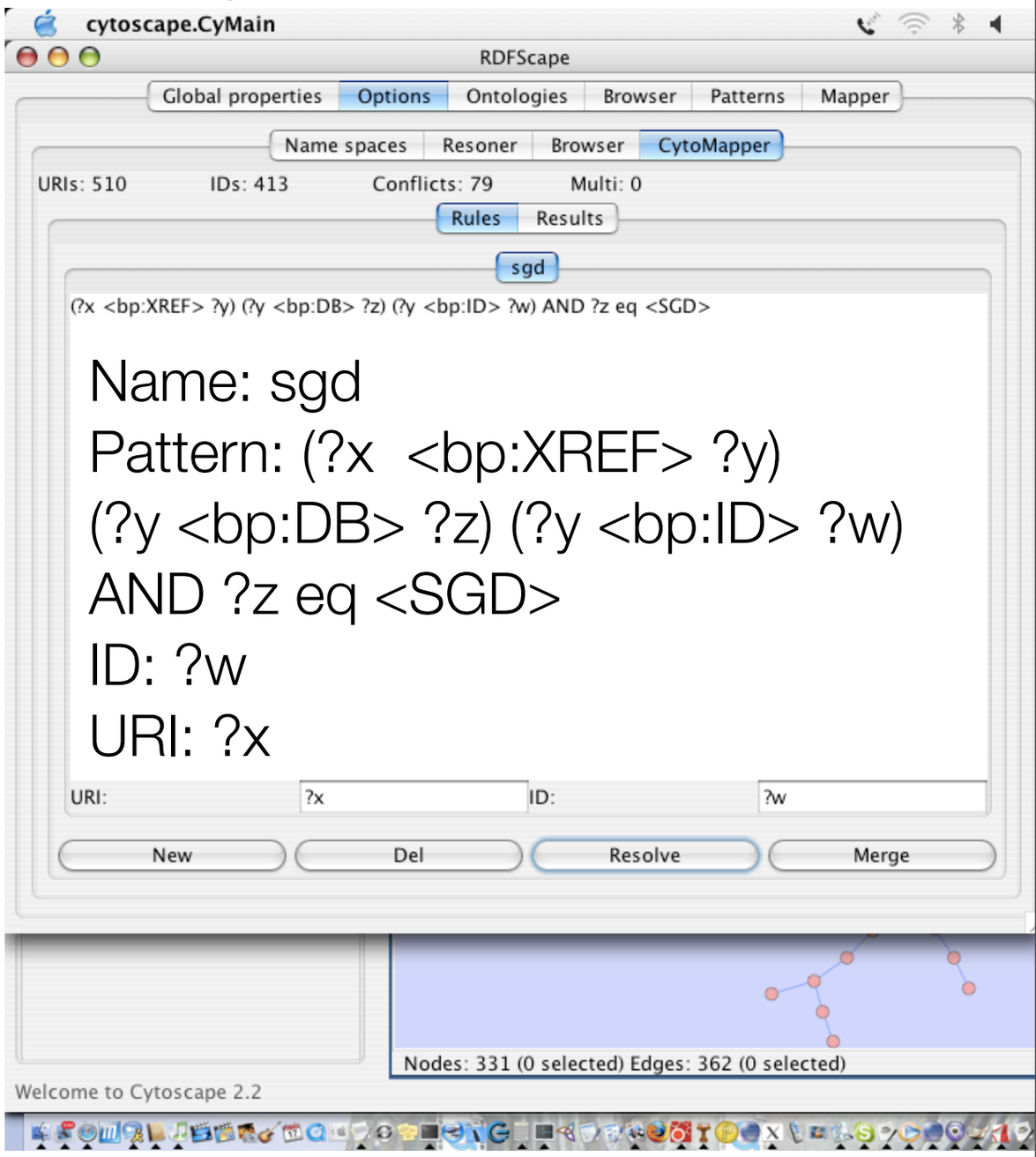
The user open a correlation network in Cytoscape, and this is connected (through RDFScape) to ontologies

Analysis

(Ontologies and data)



Defining the mapping



Analysis

(Queries on ontologies and data)

RDFScape

4) Query and browse ontologies | Pattern library | Map ontologies on my network

1) Select an analysis type! | 2) Load ontologies | 3) (optional) configure options

Browse mode

SPARQLQuery

Network

Create new network

Pattern definition

Make Editable | Get Pattern

SPQRL 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) }
```

Make Query | Clear Query | Select All | Plot Selection | Search Selection

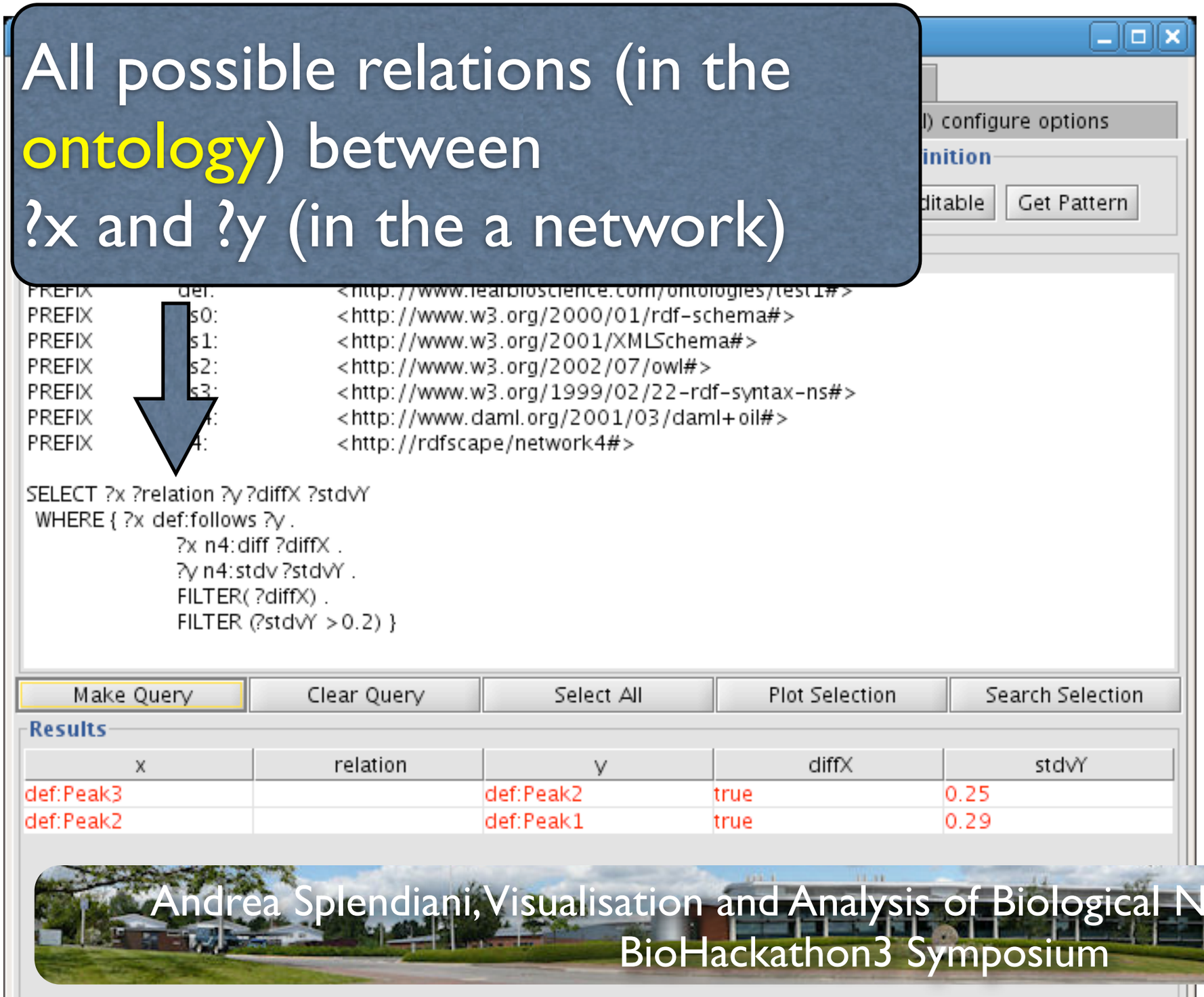
Results

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)



Analysis

(Queries on ontologies and data)

All possible relations (in the ontology) between
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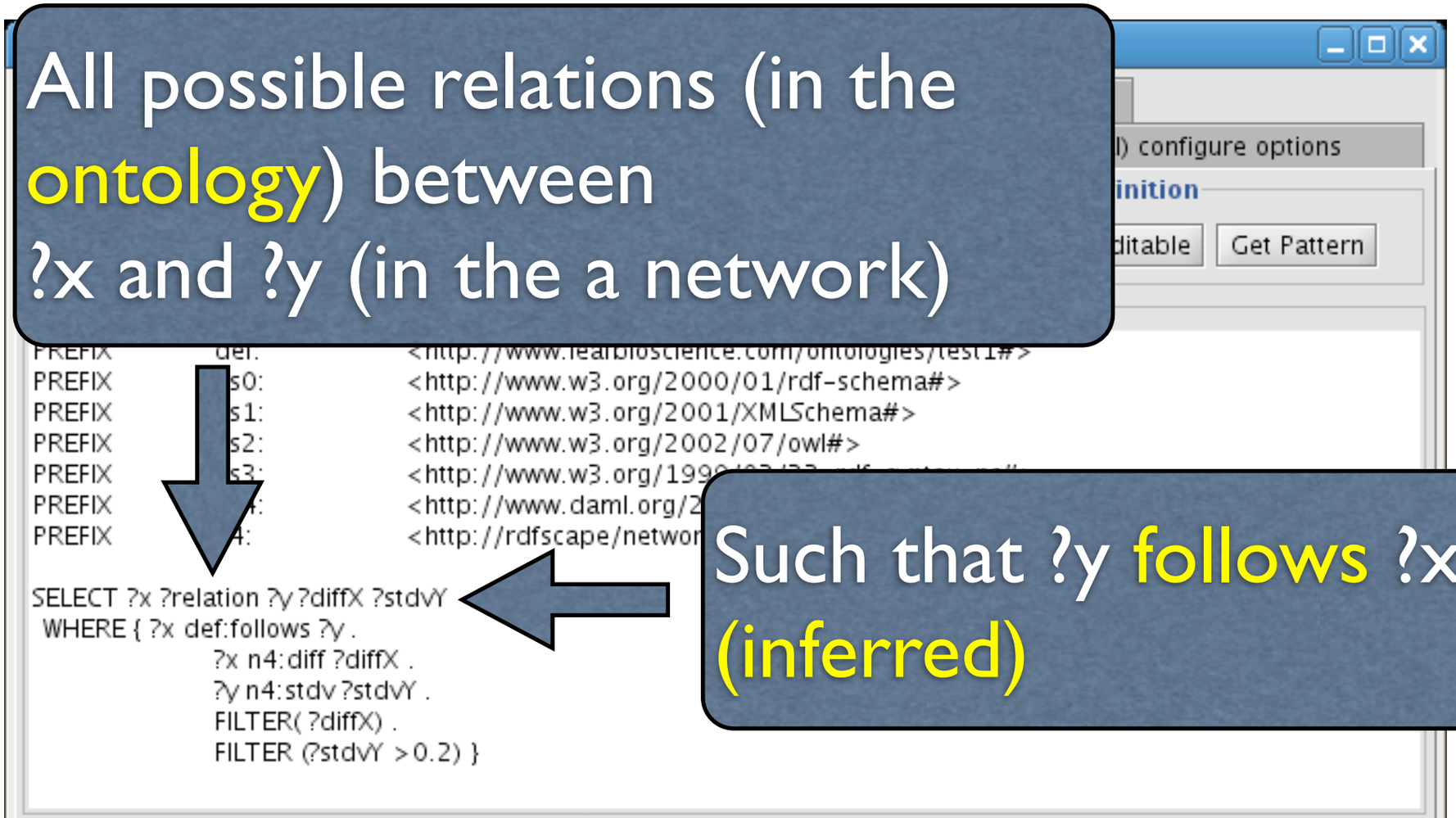
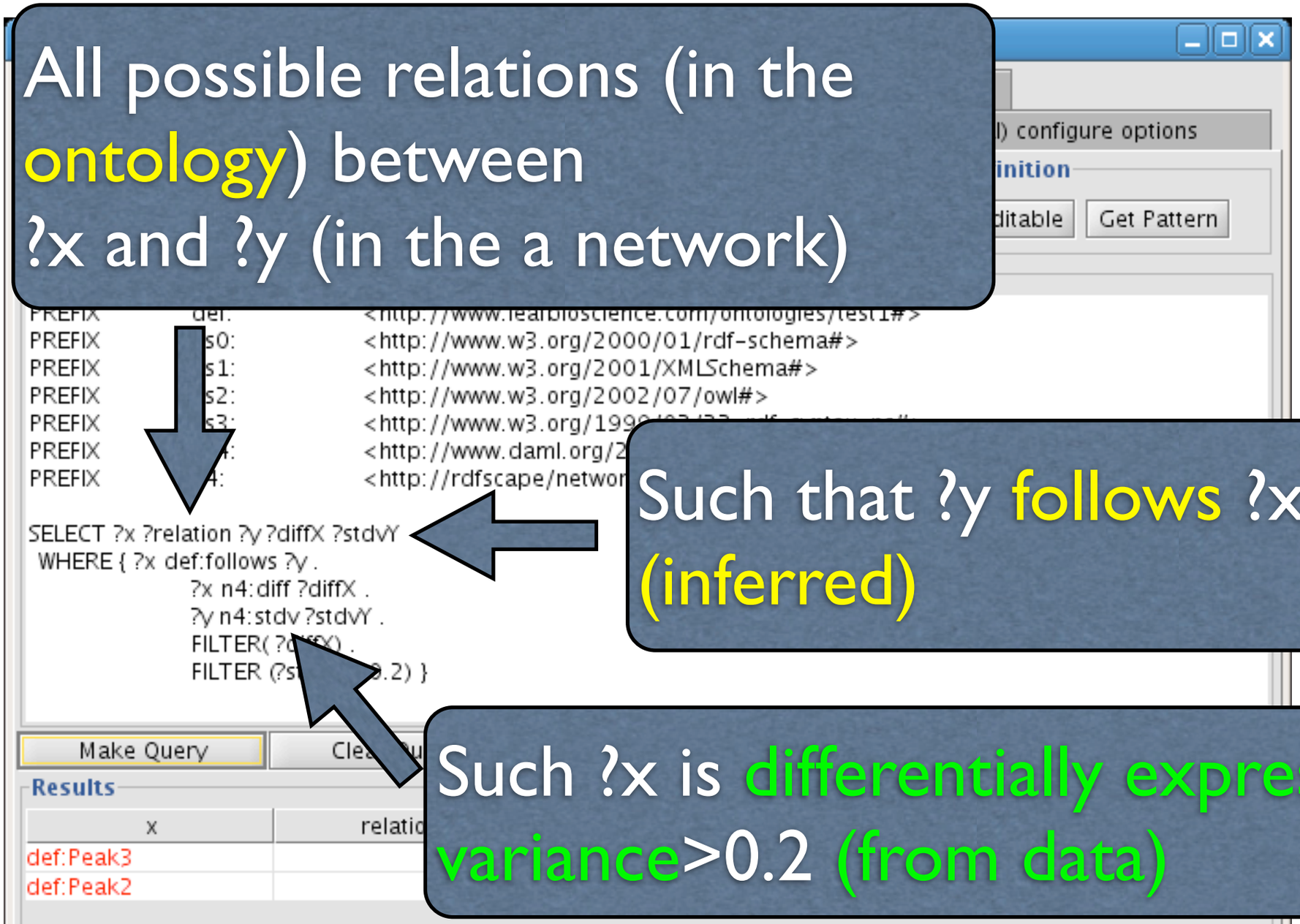


Such that ?y follows ?x
(inferred)

Analysis

(Queries on ontologies and data)

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

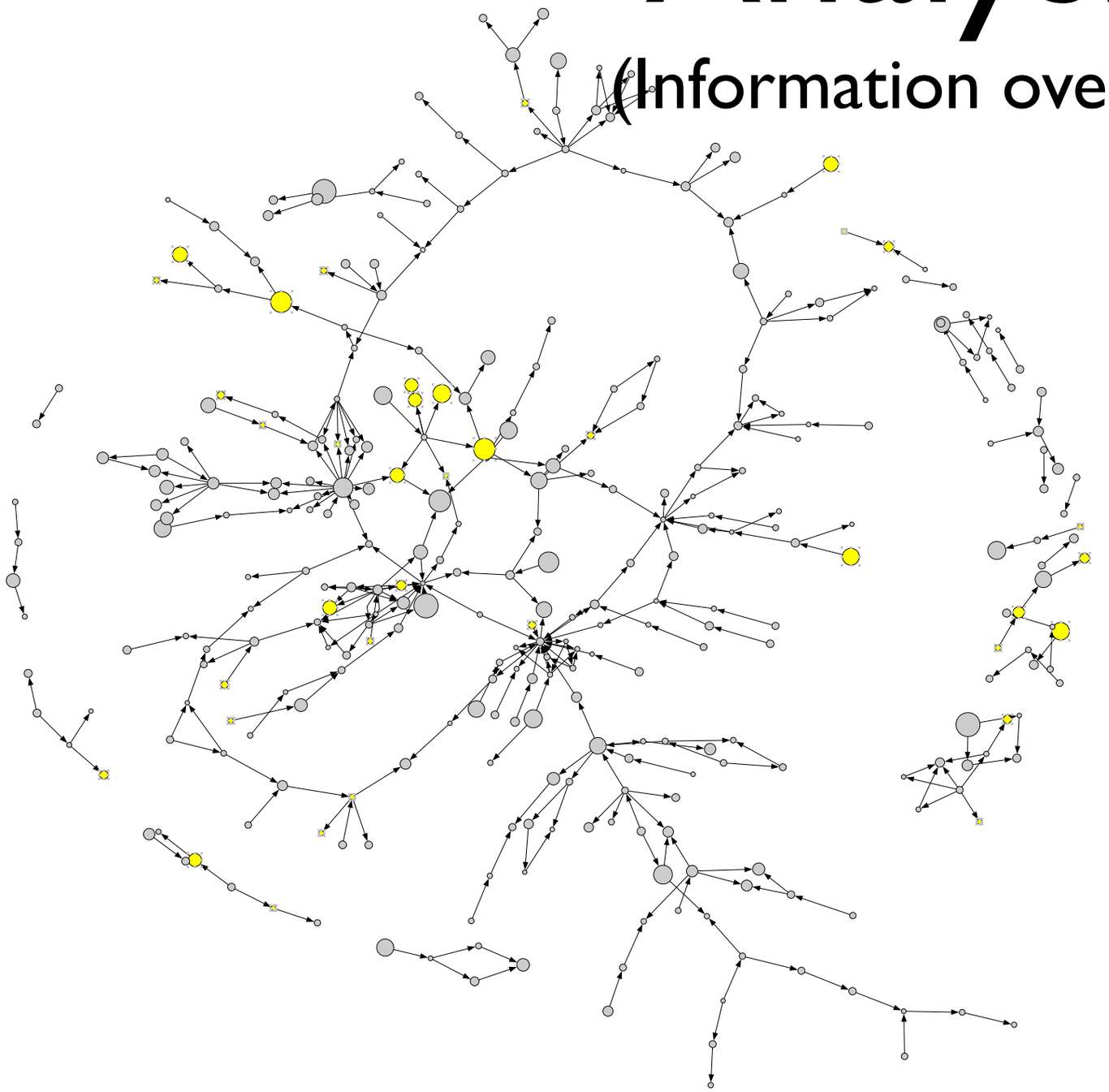


Such that ?y follows ?x
(inferred)

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

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

(Using ontologies for data analysis)

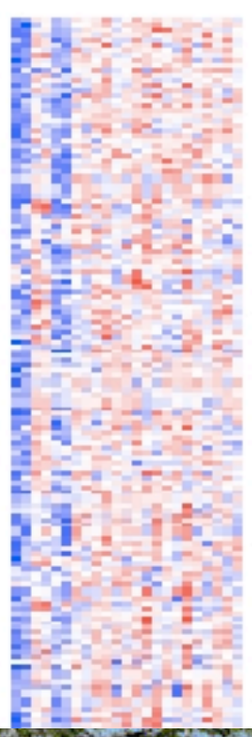
VisHiC

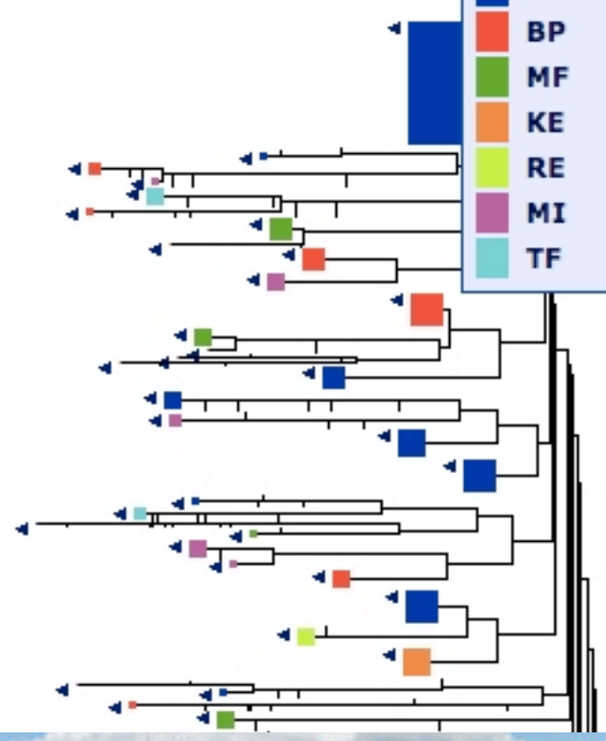
HOME >> DATASET ANALYSIS
HeLP

DATASET: GDS1023 HEMATOPOIETIC STEM CELL ENGRAFTMENT IN GOAT

Search for particular genes:

search!





Cluster id: 43674
Cluster score: 1.02E1
Size: 64

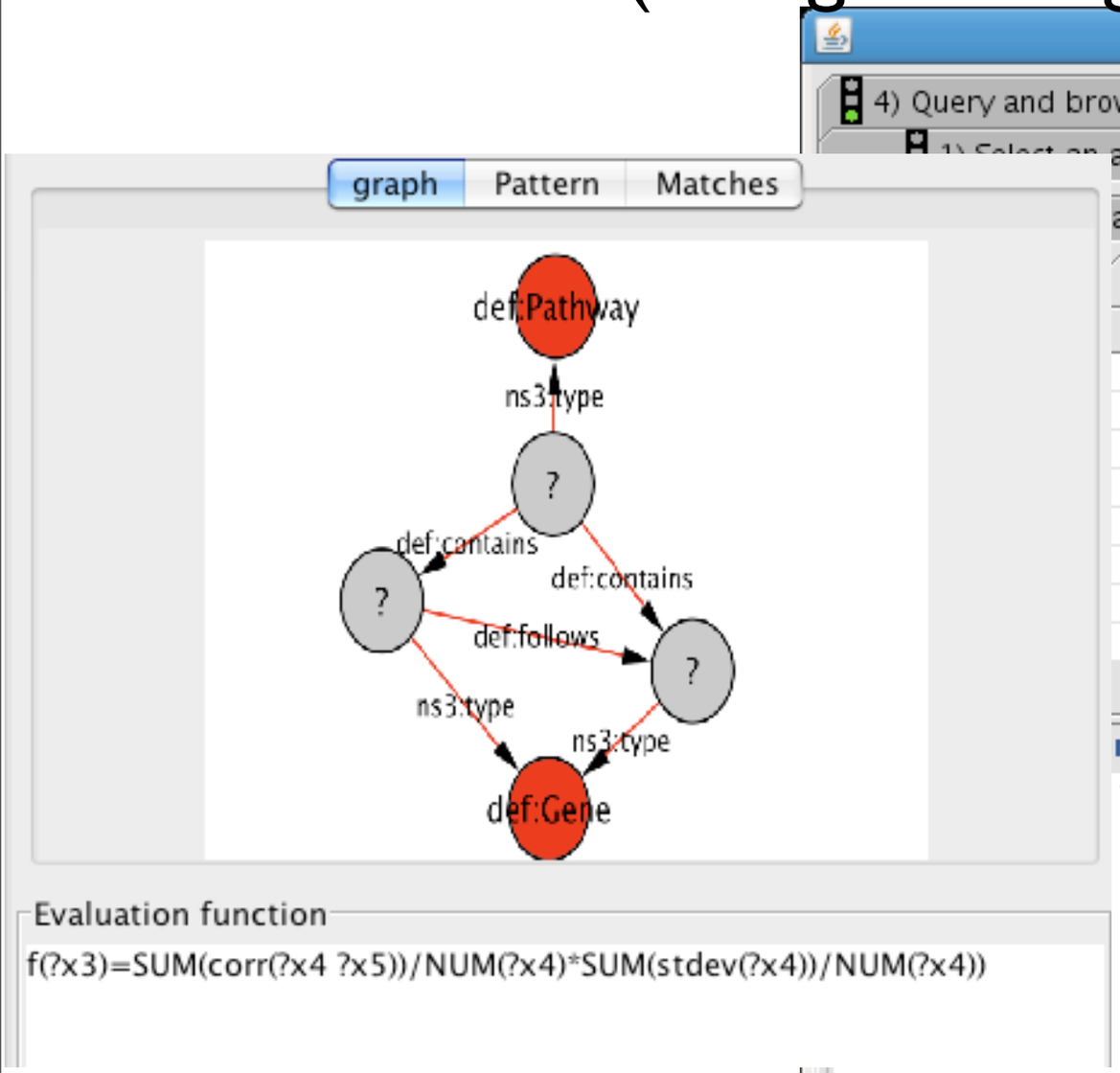
Domains Top Annotations

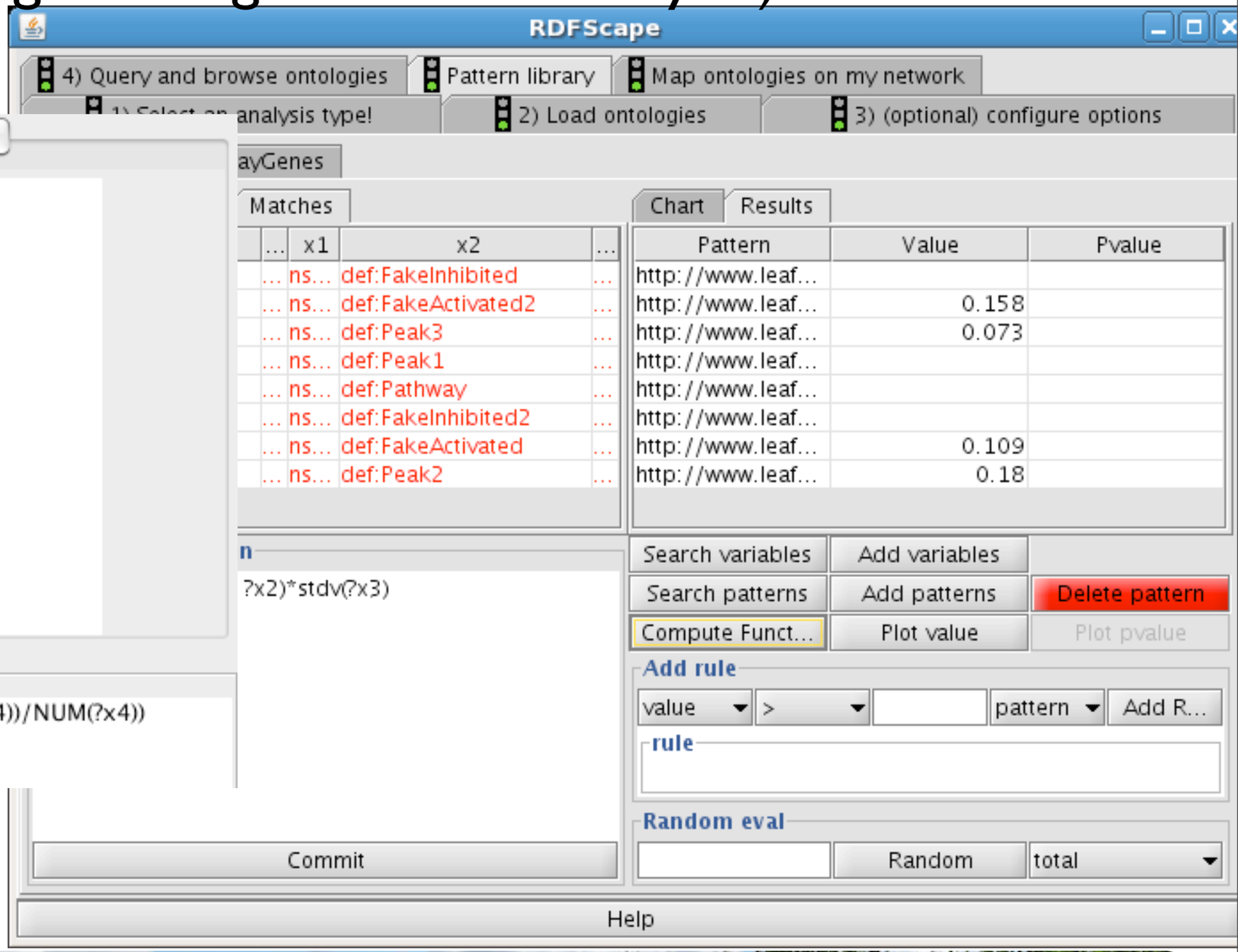
Domain	Name	Description	p-value
CC	GO:0005955	calcineurin complex	6.59E-6
BP	**GO:0008633**	**activation of pro-apoptotic gene products**	**1.4E-6**
MF			
KE	KEGG:04210	Apoptosis	2.14E-5
RE	REAC:111447	Activation of BAD and translocation to mitochondria	1.11E-4
MI			
TF			

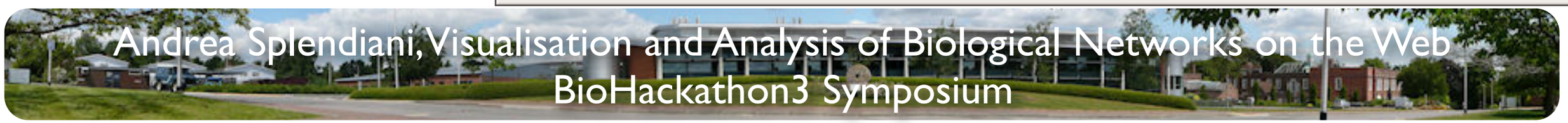
Source:
http://biit.cs.ut.ee/vishic/

Analysis

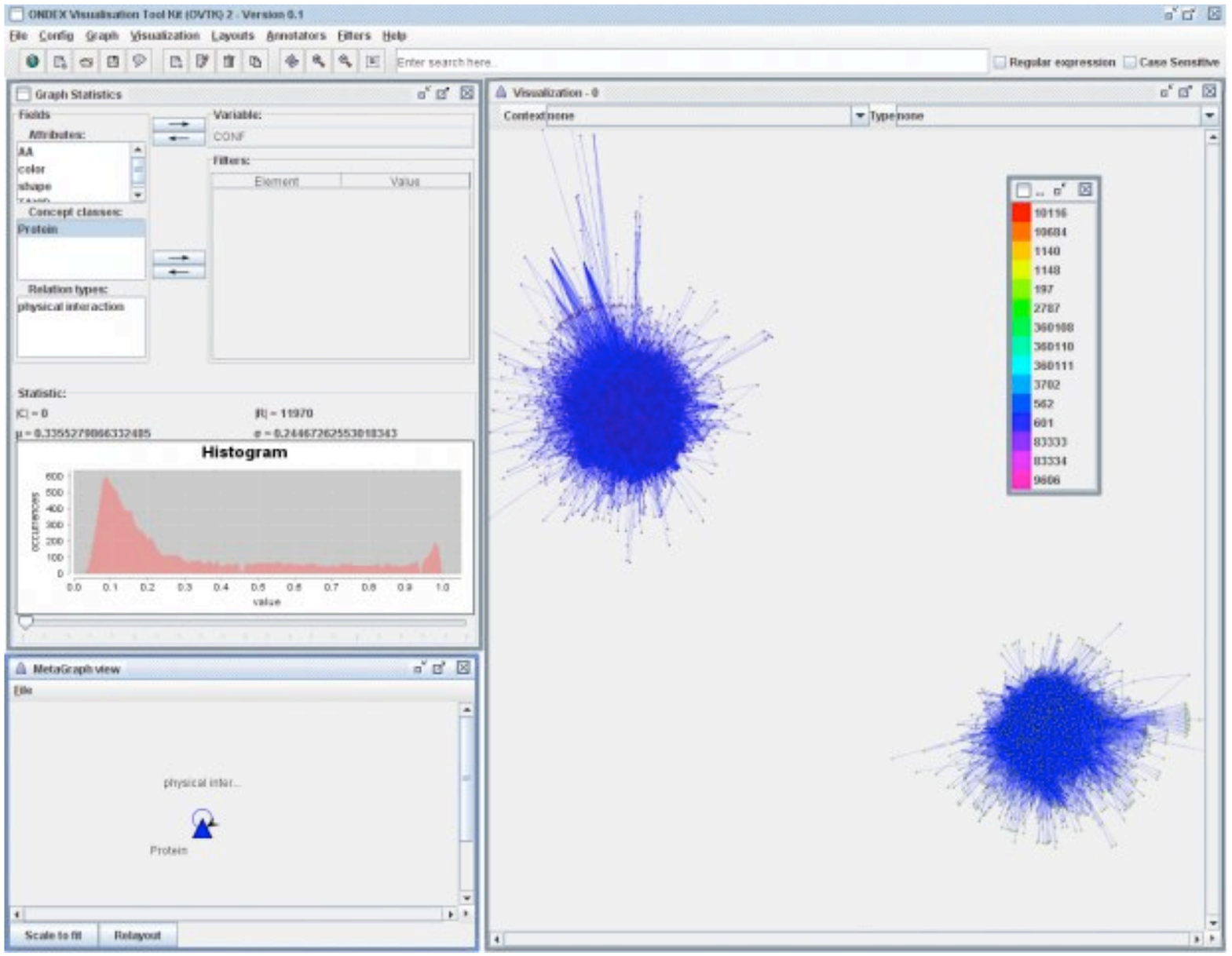
(Using ontologies for data analysis)







Analysis



Source:
http://ondex.org/

Can generic analysis tools be brought on the Semantic Web ?

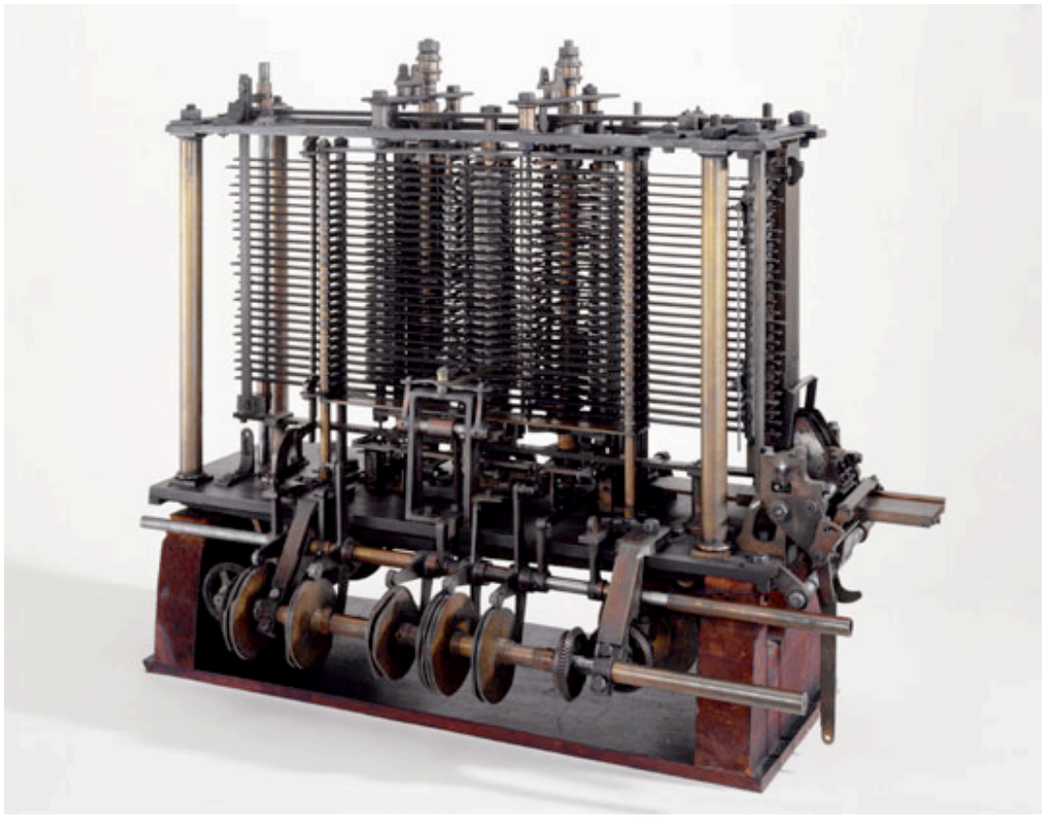
Conclusions

@Hackathon

RDFScape:
Interaction+Query+Mapping+Reasoning+Analysis=
Interface

Conclusions
@Hackathon

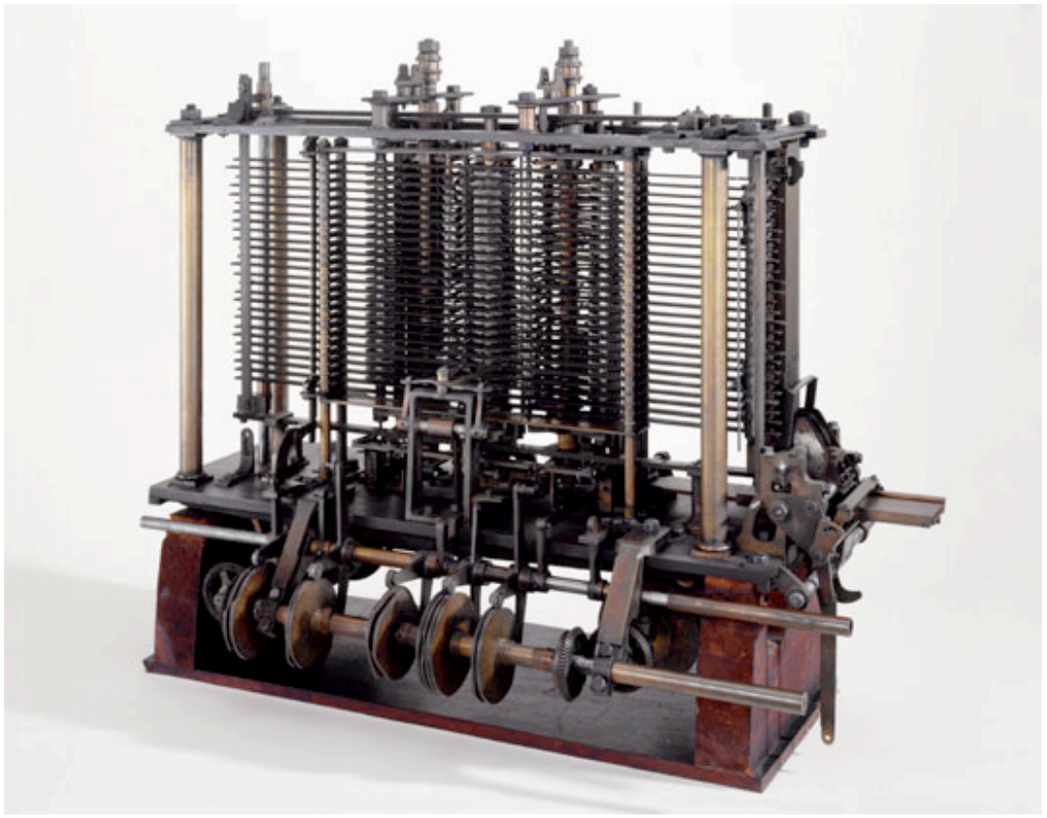
RDFScape:
Interaction+Query+Mapping+Reasoning+Analysis=
Interface



RDFScape today

Conclusions
@Hackathon

RDFScape:
Interaction+Query+Mapping+Reasoning+Analysis=
Interface



RDFScape today

RDFScape after the Hackaton

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/

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The end

Thanks