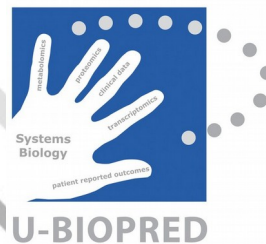




STON

Representing SBGN PD and AF in a Neo4j graph database

Vasundra Touré



- 1. Context of STON project**
- 2. Project STON : SBGN TO Neo4j**
- 3. Conclusion on STON**
- 4. Presentation of YTOS project**



Unbiased **B**IOmarkers in **P**REDiction of respiratory disease outcomes

Study Asthma

U-BIOPRED is actively supported by eTRIKS.

europaean **T**Ranslational **I**nformation and **K**nowledge Management **S**ervices

Provides a platform for translational medicine research

eTRIKS is based on the tranSMART platform.

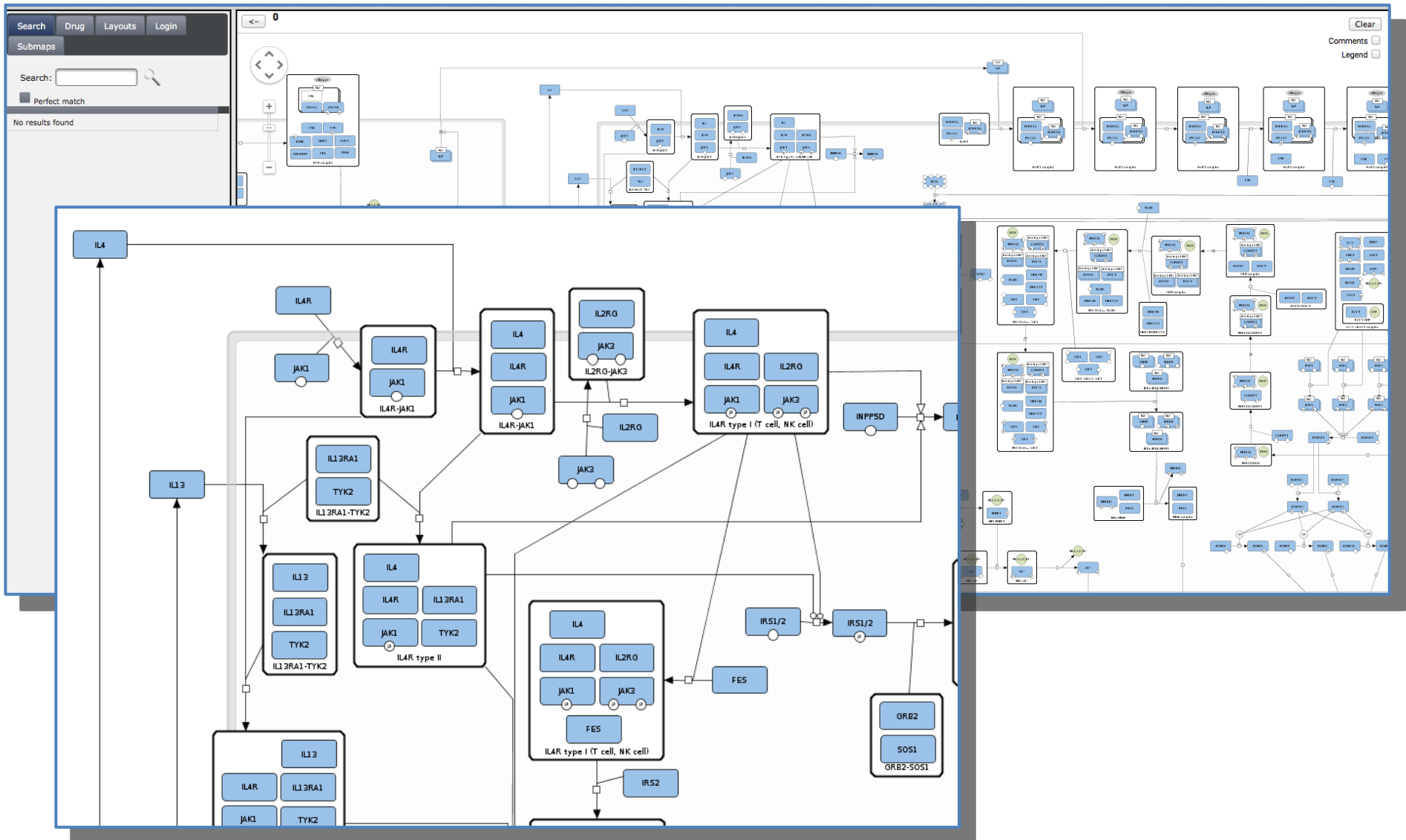


Connected
projects



The tranSMART Foundation is a global non-profit organisation. tranSMART knowledge management platform enables sharing and analysis of heterogeneous data.





Project STON : SBGN to Neo4j

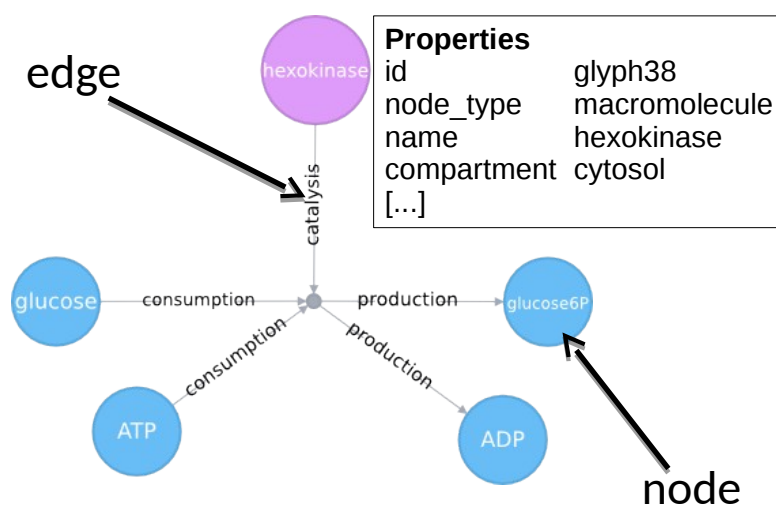
What is Neo4j ?



Neo4j graph database

NOSQL

Labeled - property



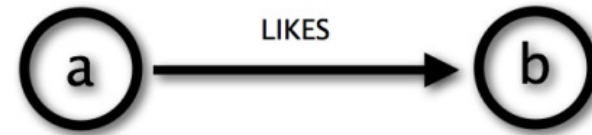
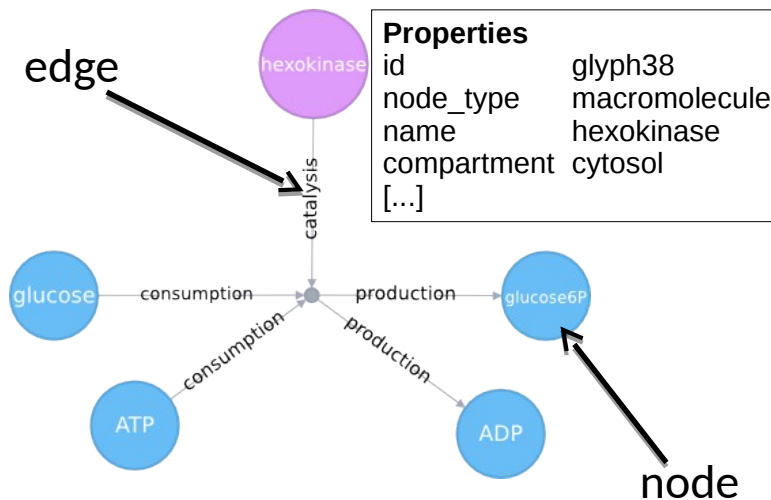
What is Neo4j ?



Neo4j graph database

NOSQL

Labeled - property



Cypher

(a) -[:LIKES]-> (b)

<http://neo4j.com/developer/cypher-query-language/>

What is Neo4j ?

localhost:7474/browser/

Rechercher

Neo4j 2.2.1

Node labels

- macromolecule
- process
- simplechemical

Relationship types

- catalysis
- consumption
- production

Property keys

- Bbox [x,y,h,w]
- Compartment
- ConsumptionPort
- FileName
- Id
- Name
- NodeType
- ProductionPort
- RelationType
- Reversible
- SbgnFileType
- SourceNodeid
- state variable
- Stoichiometry
- TargetNodeid
- unit of Information

Database

Location: /home/toure/Bureau

Query

```
$ MATCH n RETURN n LIMIT 25
```

Graph

Rows

*(25) macromolecule(7) process(5) simplechemical(13)

*(22) catalysis(5) consumption(9) production(8)

Data

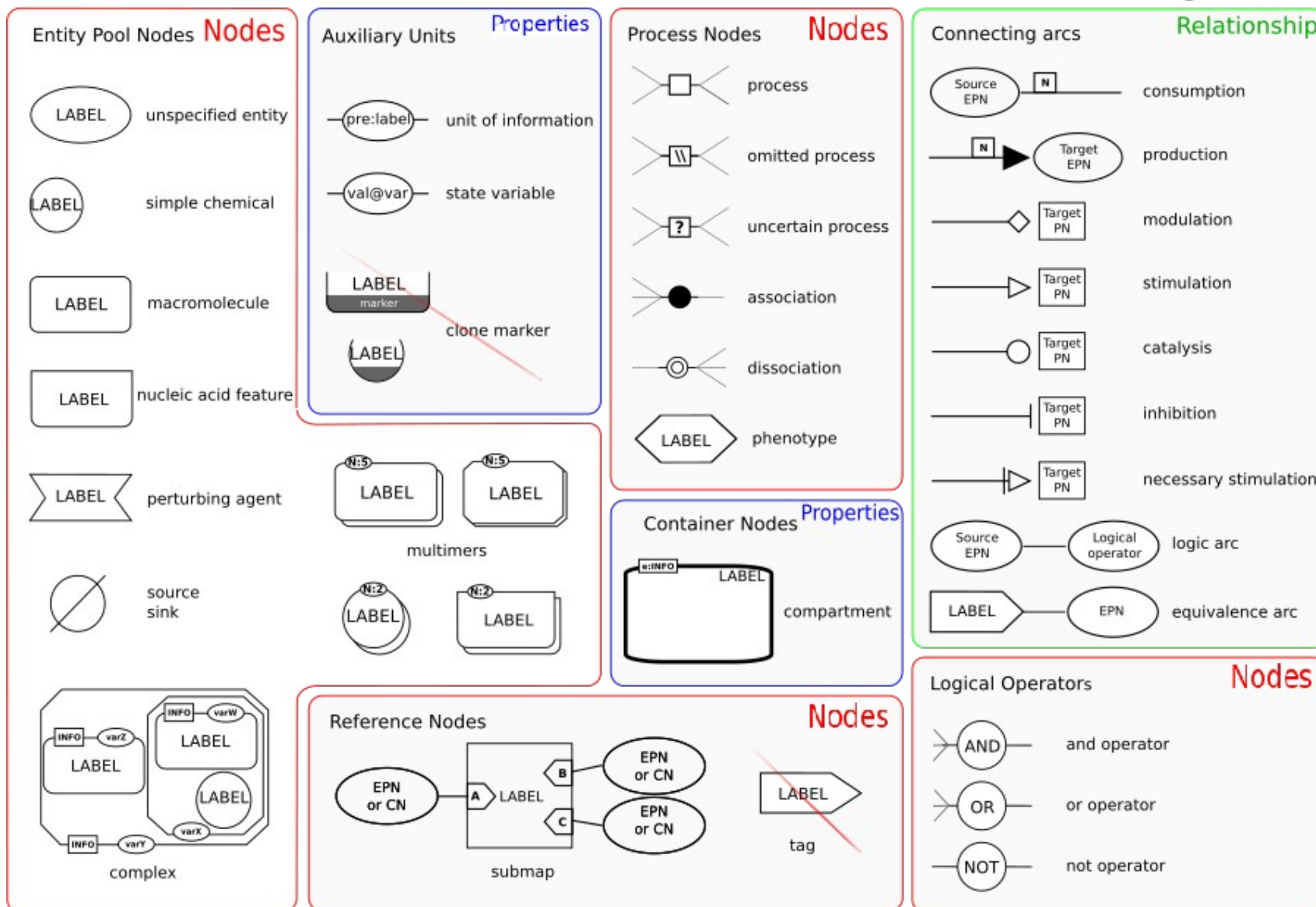
simplechemical

FileName: glycolysis SbgnFileType: processdescription NodeType: simplechemical Id: glycolysis

Name: glucose Bbox [x,y,h,w]: 90,140,60,60 Compartment: N/A state variable: unit of Information:

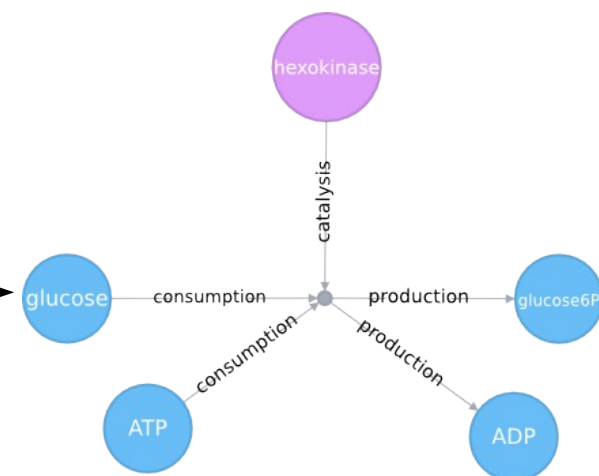
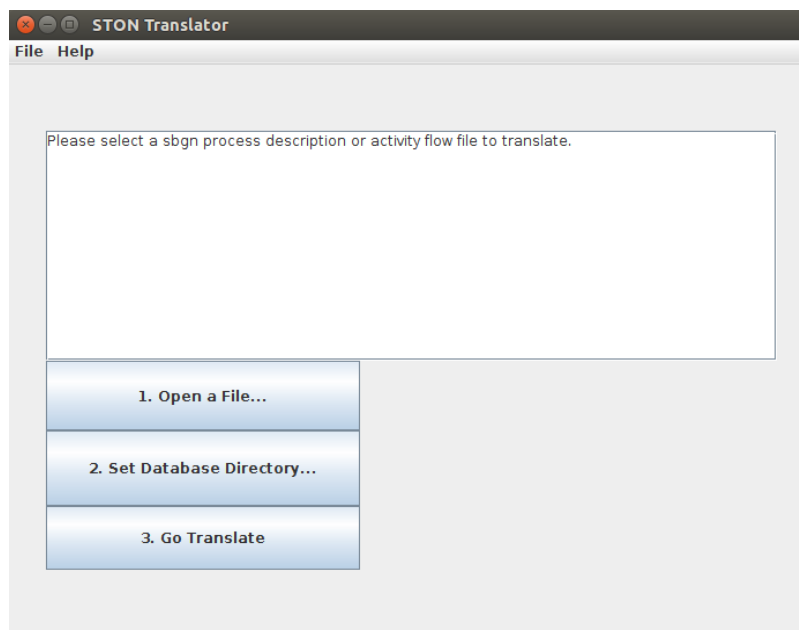
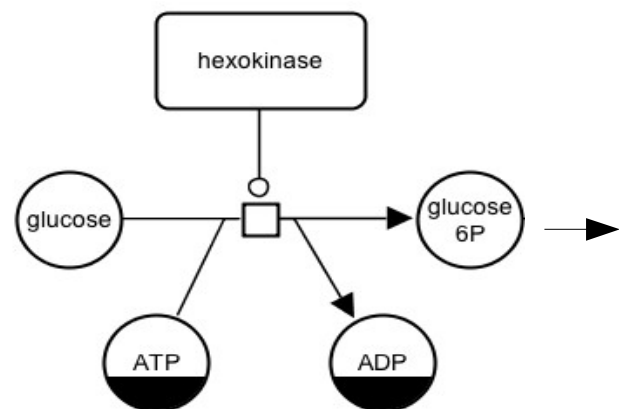
Properties

Translation rules for SBGN PD into Neo4j





PD & AF



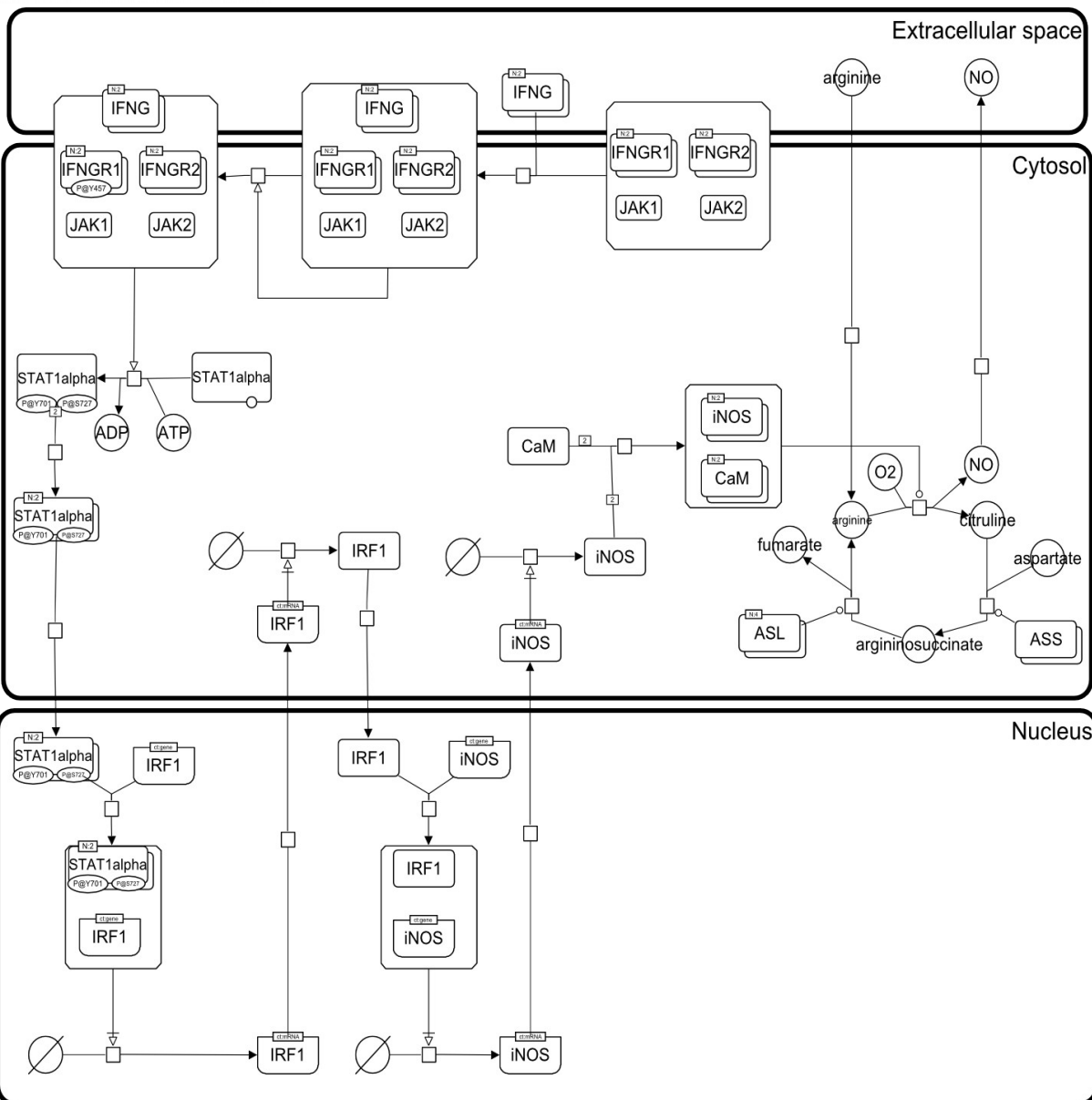
Software development

LibSBGN

Neo4j Community Edition 2.2.1

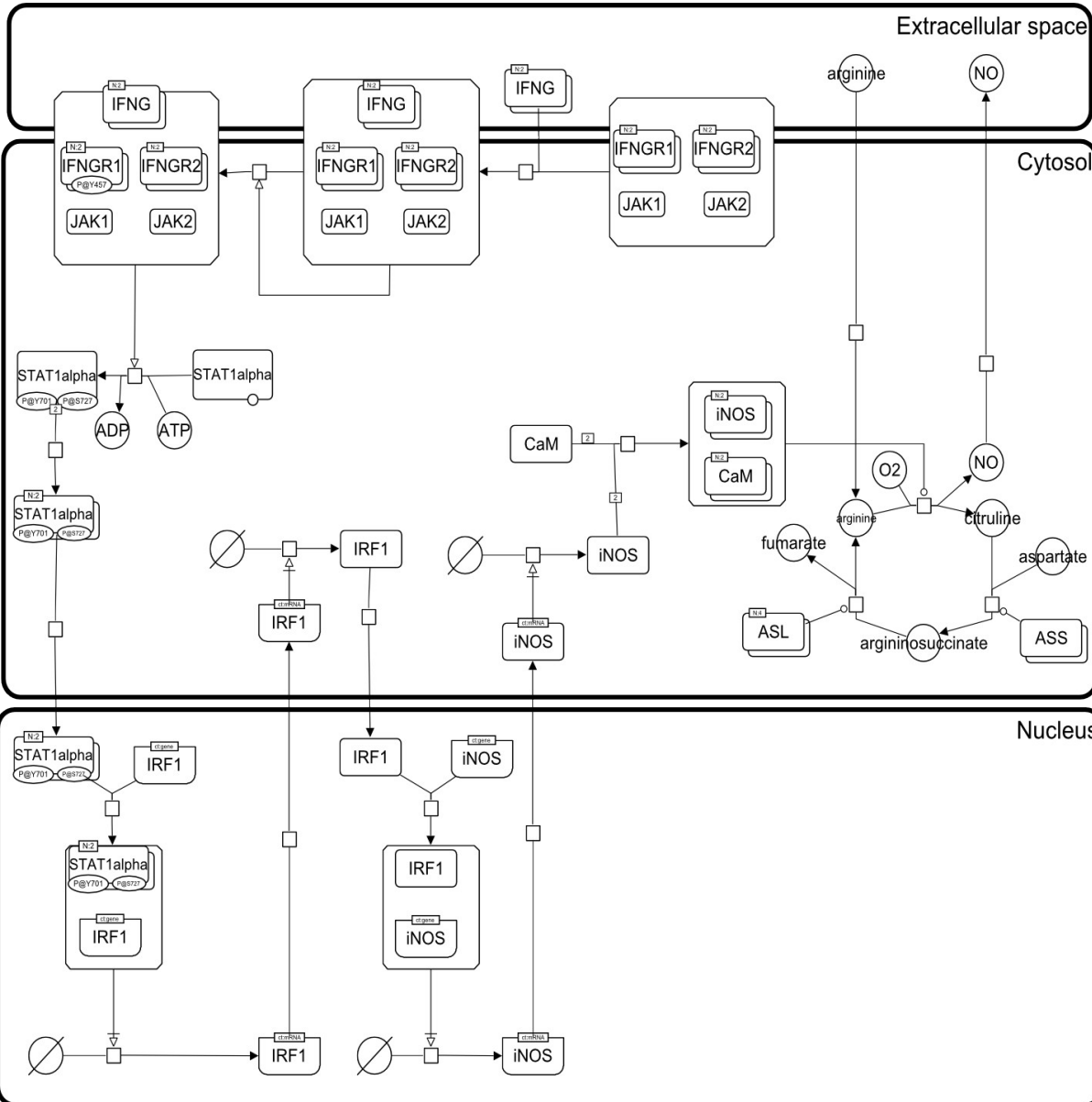
<http://sourceforge.net/projects/ston/>

Example of contribution : Finding sub-modules



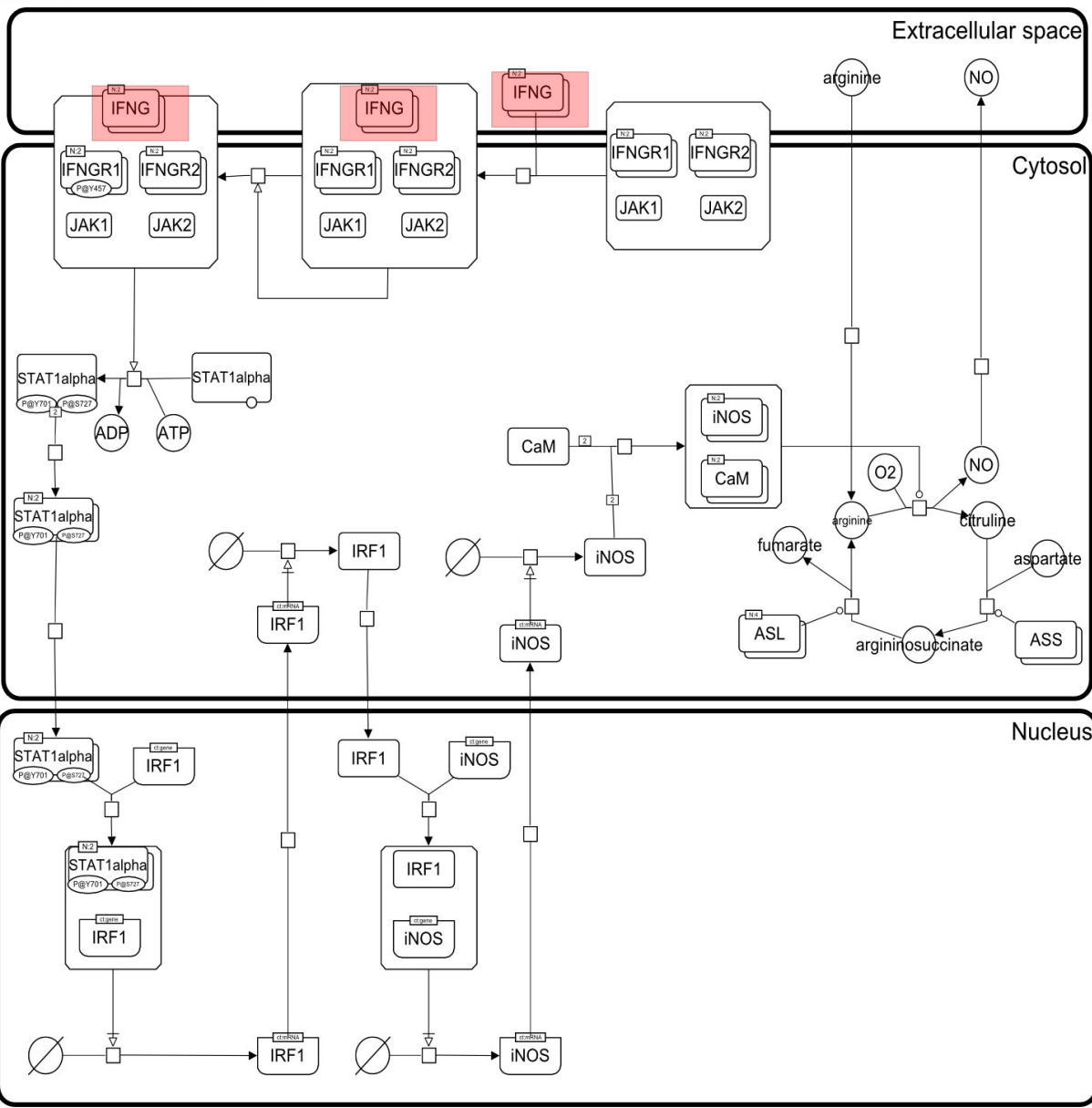
Example of contribution : Finding sub-modules

Entity of interest : **IFNG**



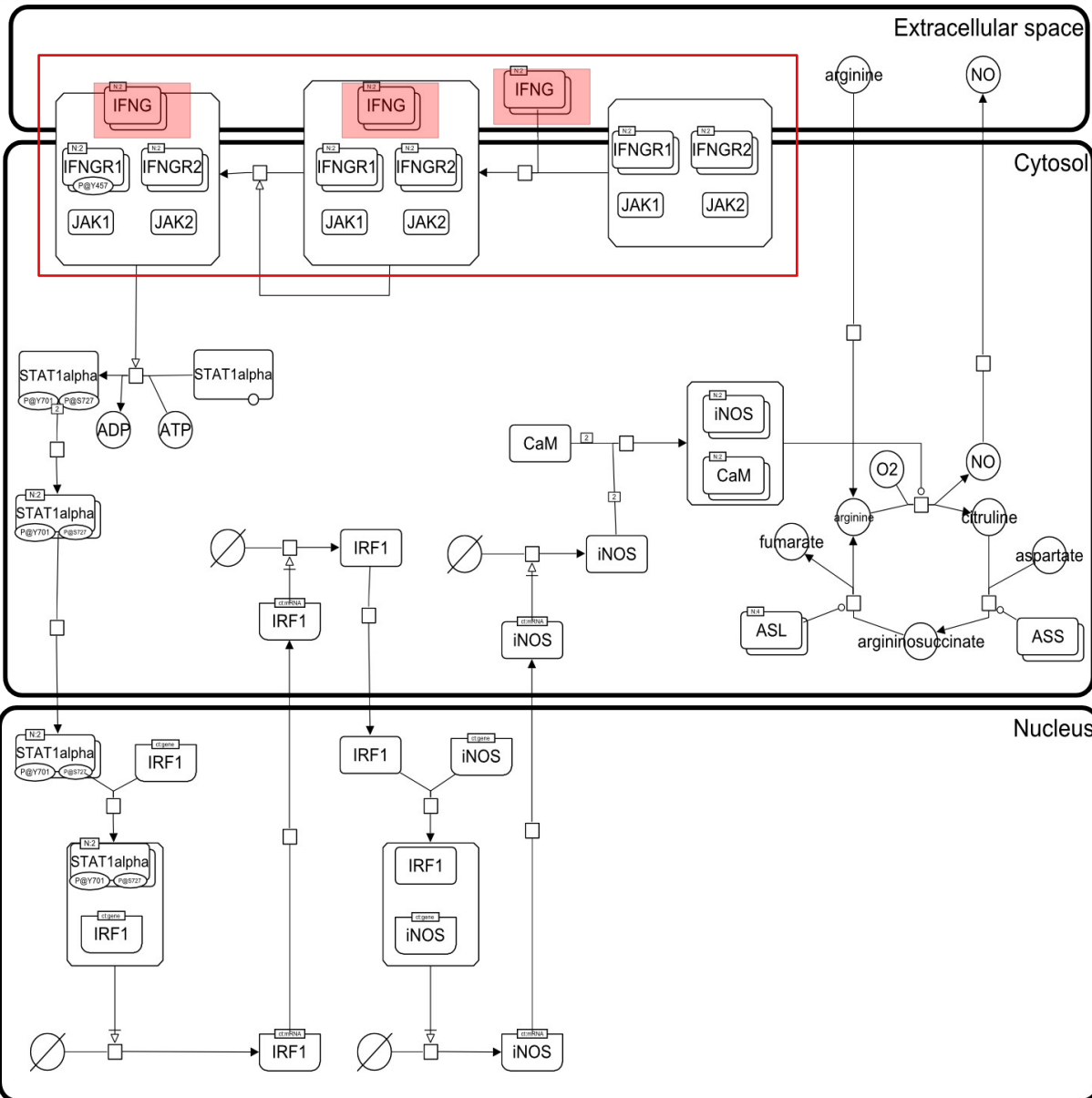
Example of contribution : Finding sub-modules

Entity of interest : **IFNG**



Example of contribution : Finding sub-modules

Entity of interest : **IFNG**

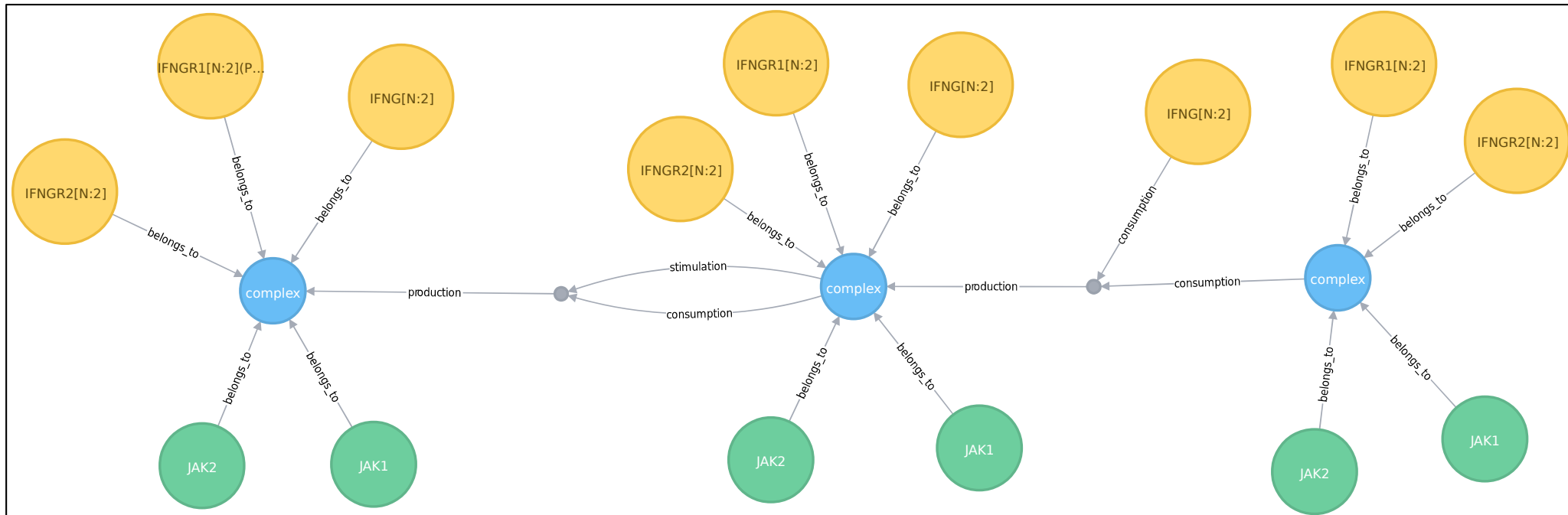


Example of contribution : Finding sub-modules

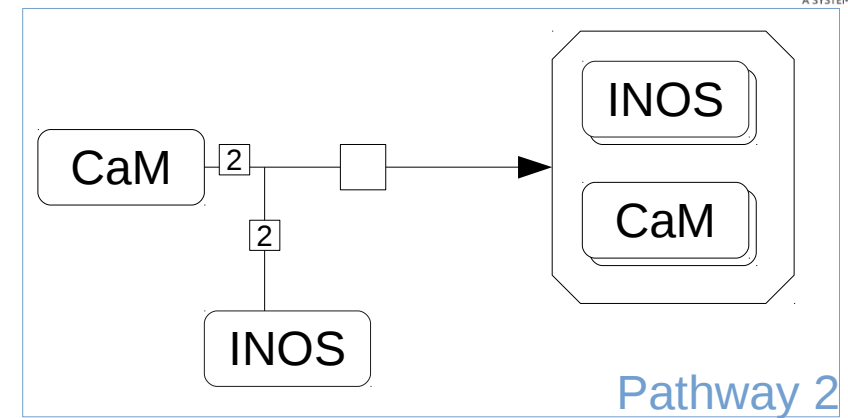
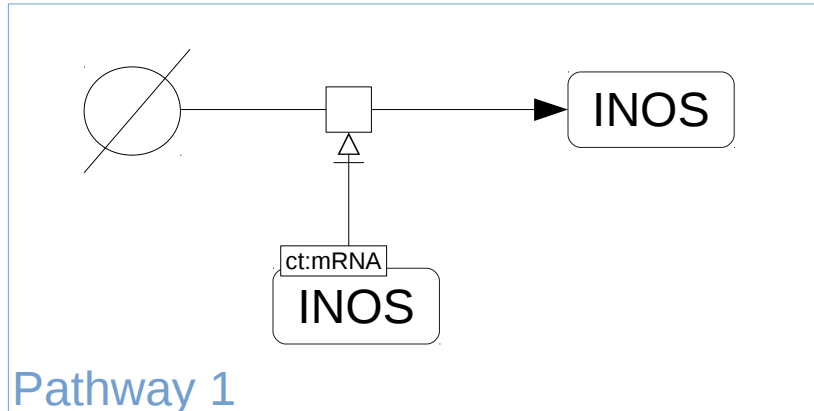
Cypher
query

```
match n-->p, x, z
where n.name = 'IFNG' and x.node_type <> 'process' and z.node_type <> 'process'
return n-->p, p-[*1]->x, z-[*1..2]->p
```

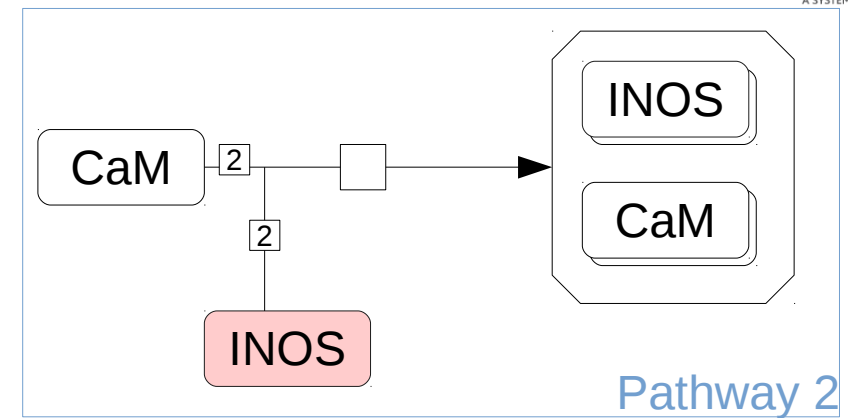
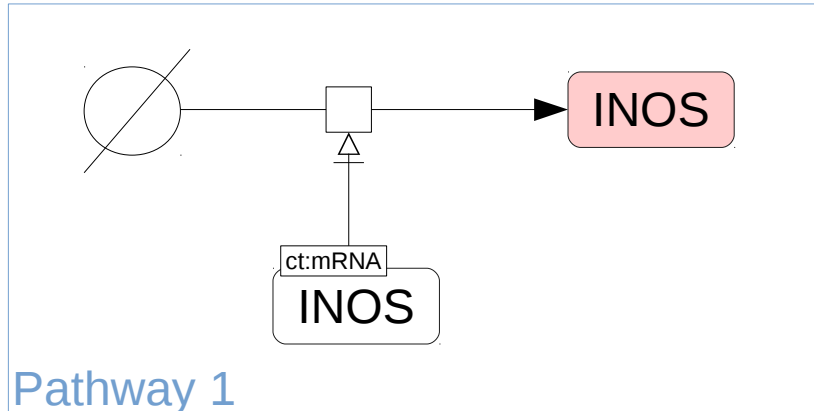
Result in Neo4j :



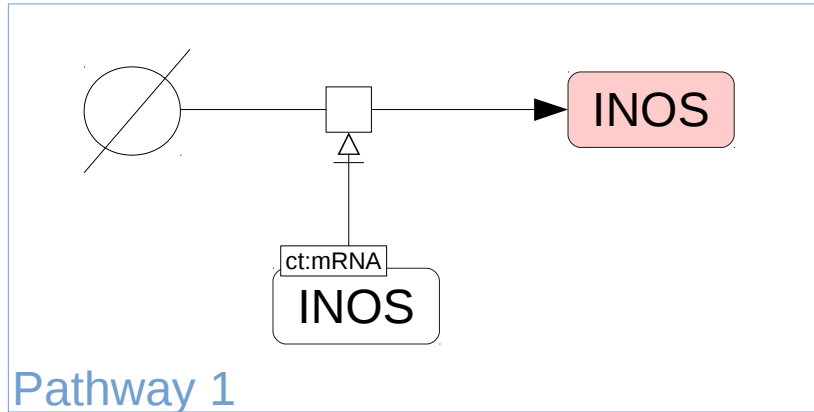
Perspectives : Combining pathways



Perspectives : Combining pathways

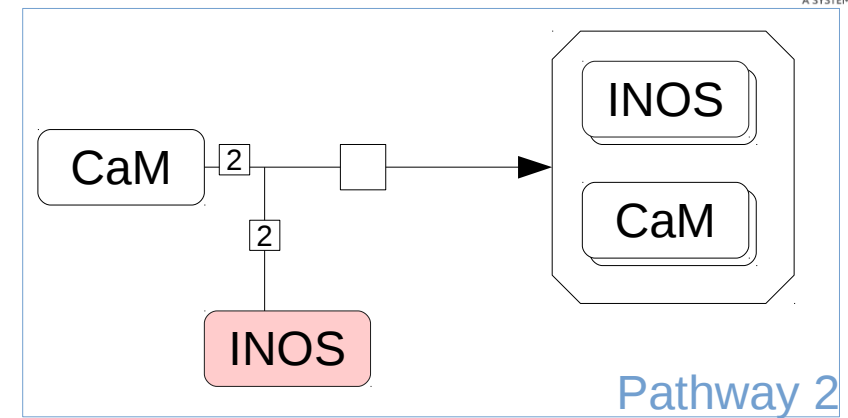


Perspectives : Combining pathways

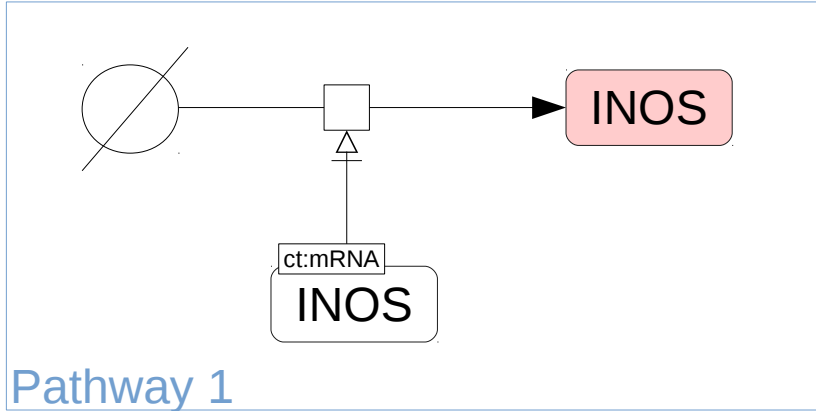


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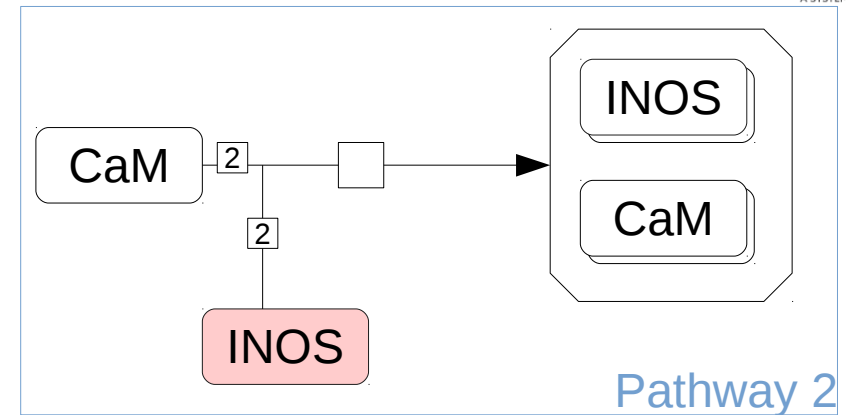
STON



Perspectives : Combining pathways

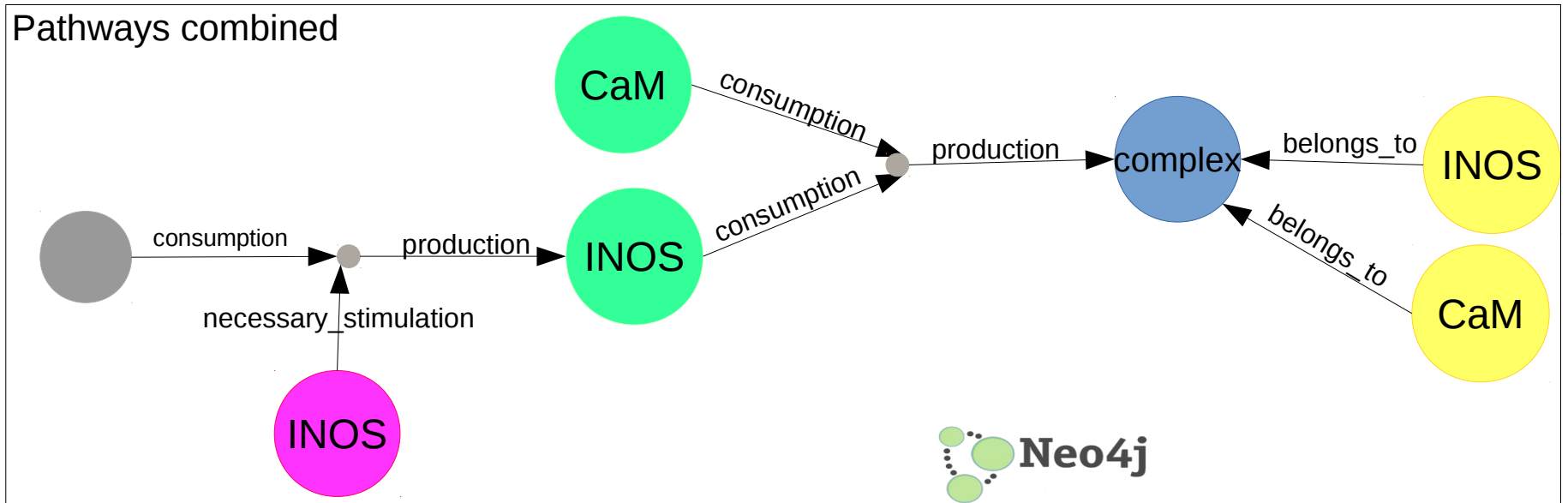


+



STON

Pathways combined



STON

Complete translation of SBGN PD & AF into Neo4j graph database

Perspectives :

- Combining pathways
- Integrate into MaSyMoS

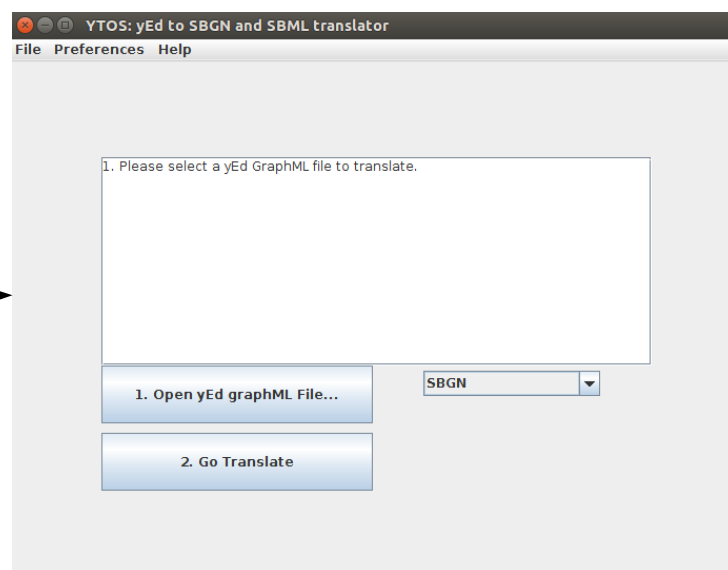
Project YTOS : yEd TO SBGN & SBML

Yed Graph Editor

Easy drawing – Good layout
Powerful zooming



Metabolic & Signalling
pathways



Software development

LibSBGN - JSBML
XML parser

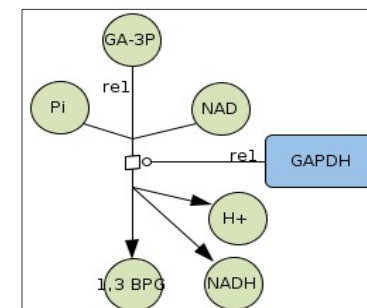
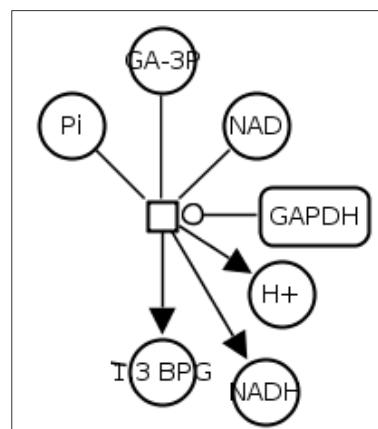
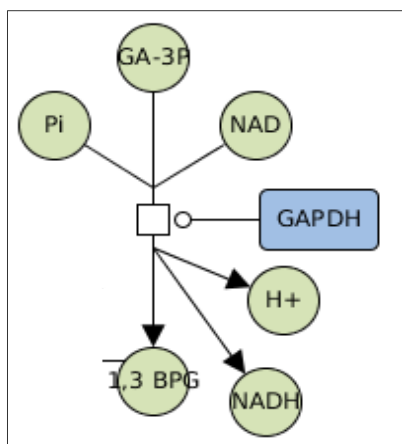
<http://sourceforge.net/projects/ytos/>



YTOS

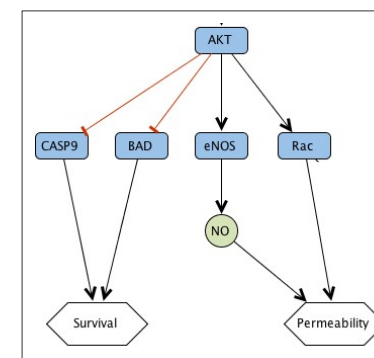
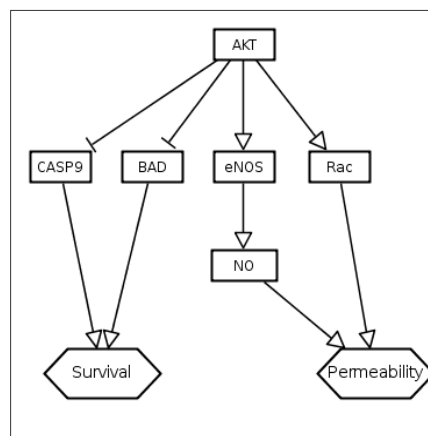
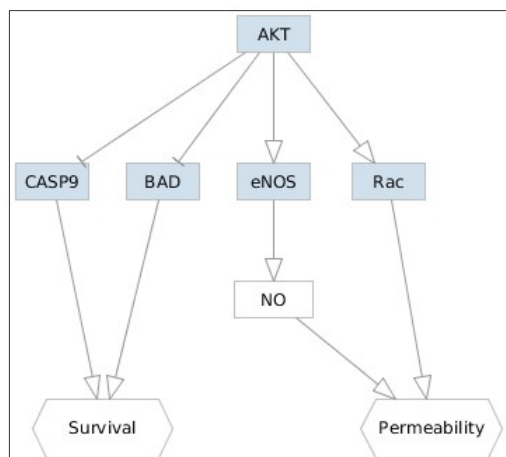


Metabolic



```
<species compartment="default" name="GAPDH" id="n28">
  <annotation>
    <celldesigner:extension>
      <celldesigner:speciesIdentity>
        <celldesigner:class>PROTEIN</celldesigner:class>
        <celldesigner:proteinReference>pr22</celldesigner:proteinReference>
      </celldesigner:speciesIdentity>
    </celldesigner:extension>
  </annotation>
</species>
```

Signaling / AF



A special thanks to:



Dr. Alexander Mazein

Dr. Dagmar Waltemath

Pr. Christine Froidevaux

Dr. Irina Roznovat

Ron Henkel

Johann Pellet

Dr. Mansoor Saqi

Pr. Charles Auffray

Financial support :



Manuscripts in preparation:

- Touré V, Mazein A, Roznovat I, Waltemath D, Henkel R, Saqi M, Pellet J and Auffray C: **STON, SBGN to Neo4j: Representation of Systems Biology pathway as graph-oriented models**. 2015. In preparation. Target journal: BMC Systems Biology.
- Touré V, Mazein A, Roznovat I, Saqi M, Pellet J and Auffray C: **YTOS, yEd to SBML and SBGN: Adapting metabolic pathways developed with general-purpose yEd graph editor to Systems Biology standards**. 2015. In preparation. Target journal: Journal of Computational Biology.