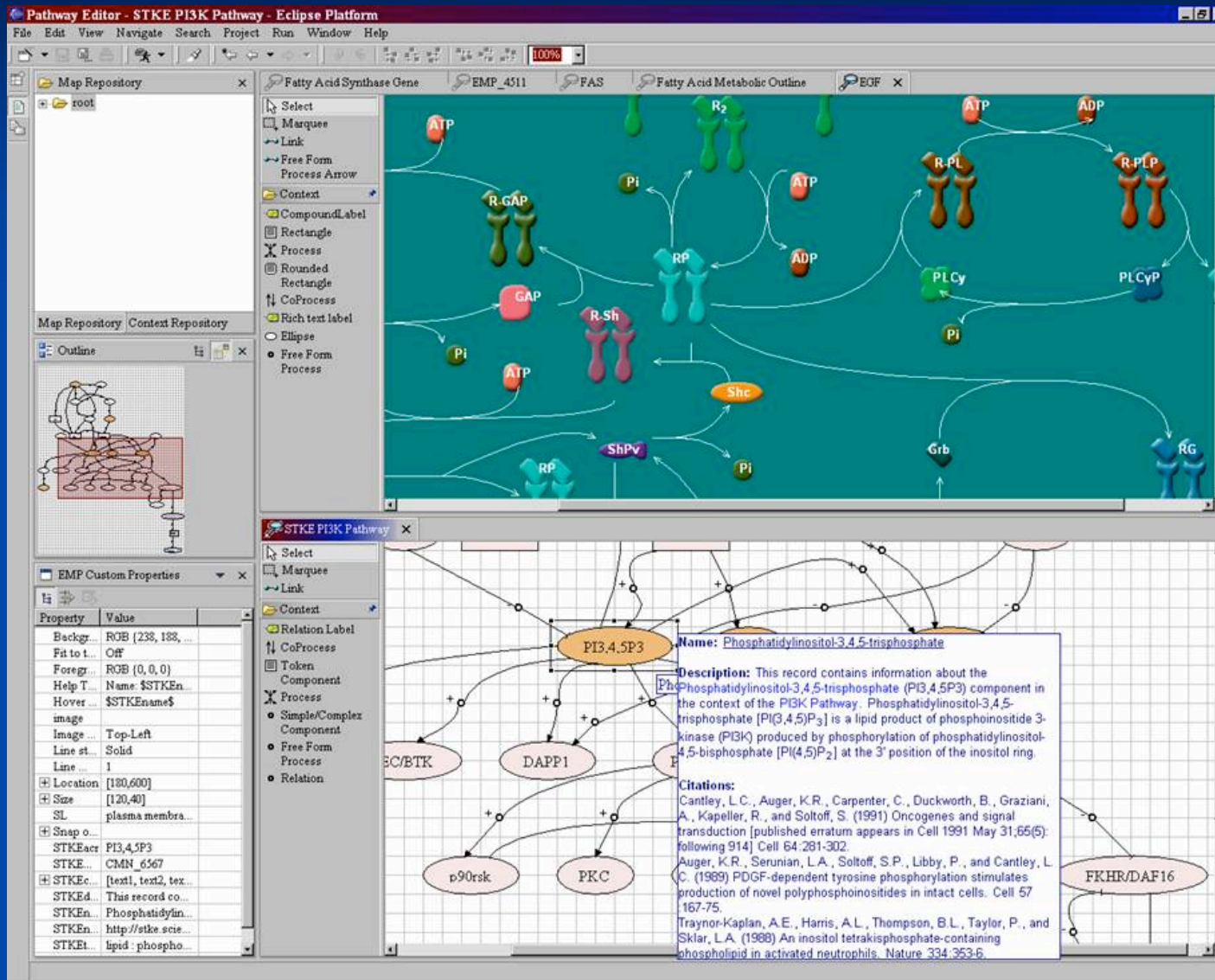# Edinburgh Pathway Editor

a flexible tool for biological model creation

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Edinburgh Centre for Bioinformatics

Edinburgh Pathway Editor

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History of the notation

- EMP/MPW   (1990)
- WIT (2000)
  - Puma 2 compbio.mcs.anl.gov/puma2/cgi-bin/met_recon.cgi
  - GeneGo
  - SEED
- Edinburgh Pathway Editor www.bioinformatics.ed.ac.uk/epe/

Basic features

- Eclipse-based open plug-in design
- Metadata-oriented design
- Small number of basic objects to represent main concepts of the biological network
- Flexible visual presentation
- Internal RDBMS storage
- XML-based internal presentation
- Flexible export facility

Model export

- Built-in SBML-1 export of metabolic networks
- Extended XPath based API for SBML-2 export of predefined contexts
- Internal XML representation for backup and data exchange
- Export map as list of chemical reactions
- Export of whole folder tree to the HTML
- Save diagrams in standard graphic formats (JPG,PNG,PNG)

Eclipse open architecture

- Extension of basic features
  - New DBMS
  - New image format
- Implementation of domain specific features
  - Model validation rules
  - Export
  - Visualisation of new type of data (simulaton results, experimental data)

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Data storage

- Relational database storage
  - For stand-alone usage
    - Apache Derby
    - HypersonicSQL
  - For corporate usage
    - Oracle
    - MySQL

Metadata based approach

- Every map links to Context
- Context store list of object, which could be added to the map
- Every object belongs to small number of "base objects"

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Context

- Description of metadata related to the map
  - User-defined object types
  - Domain-specific object properties
  - Default values

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Base objects

- *Shape*

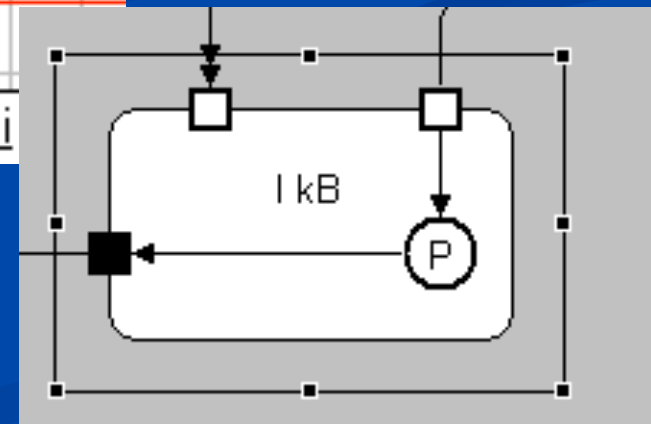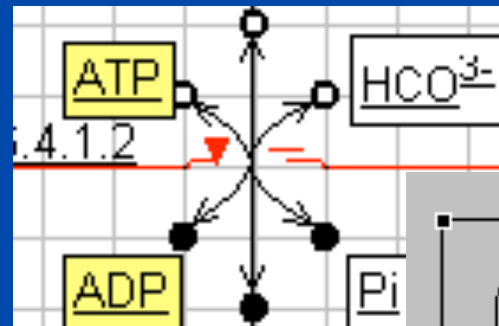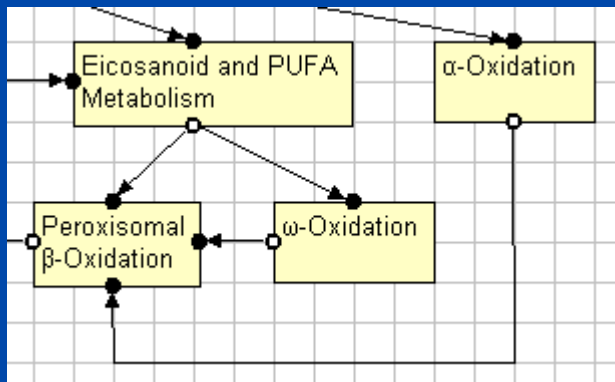- *Port*

- *Process*

- *Link*

- *Label*

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Shape

- *Shape* represents the biological object or subsystem, treated as "a black box" .
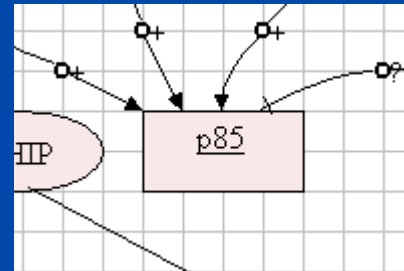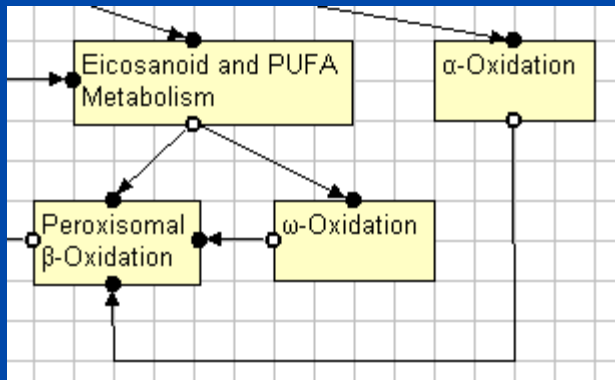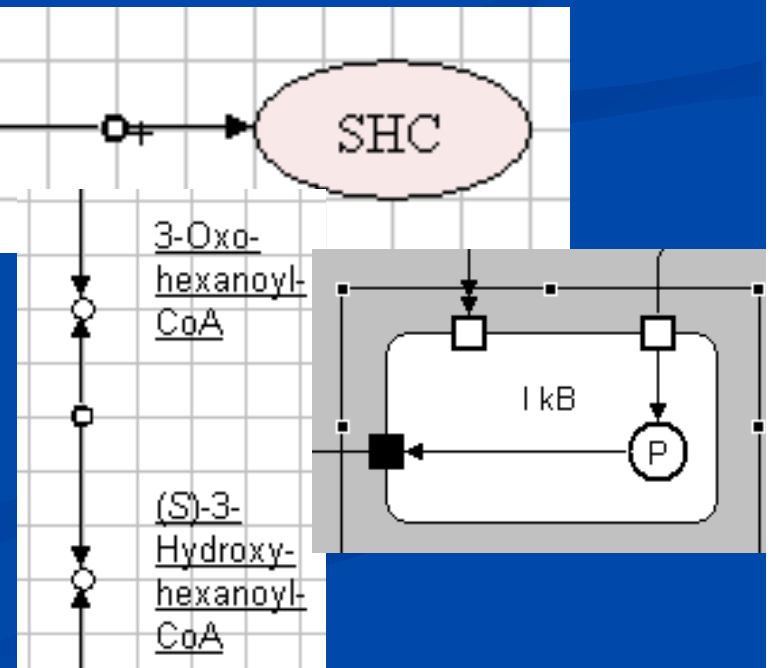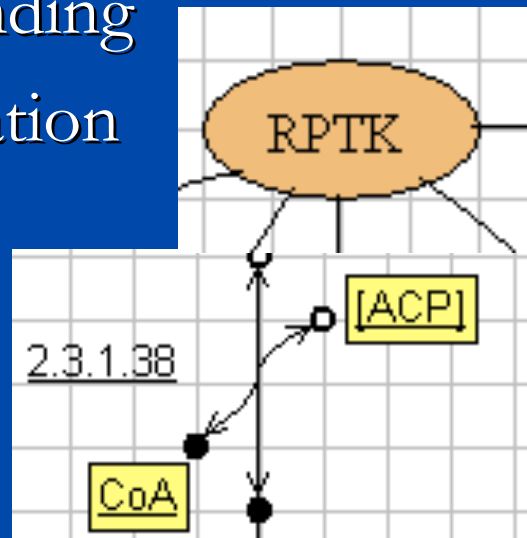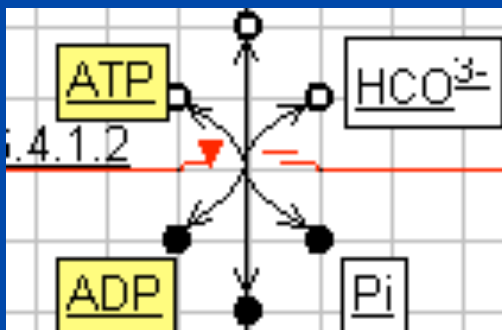
Port

- The port is used to designate the state of the object, in which it could interact with other objects. The port is the interface between the objects.
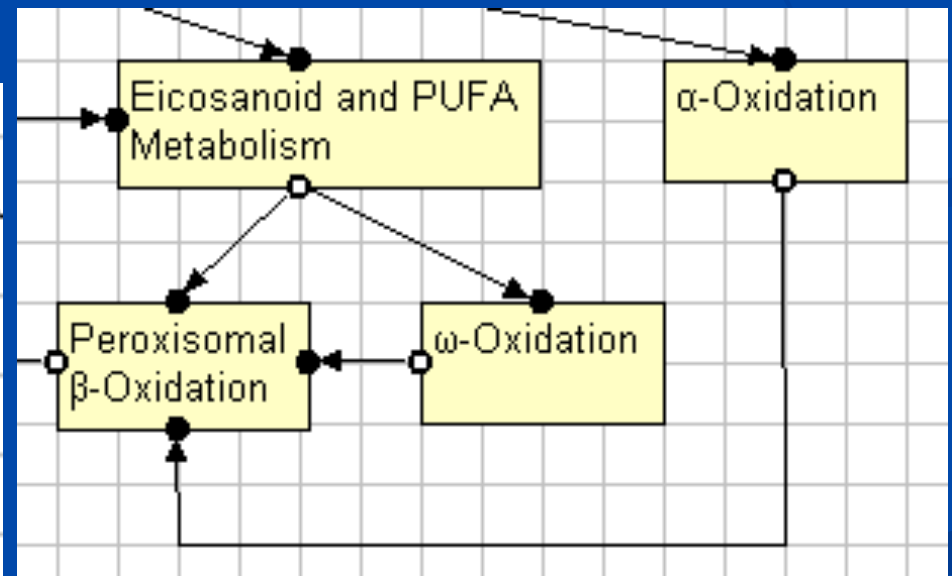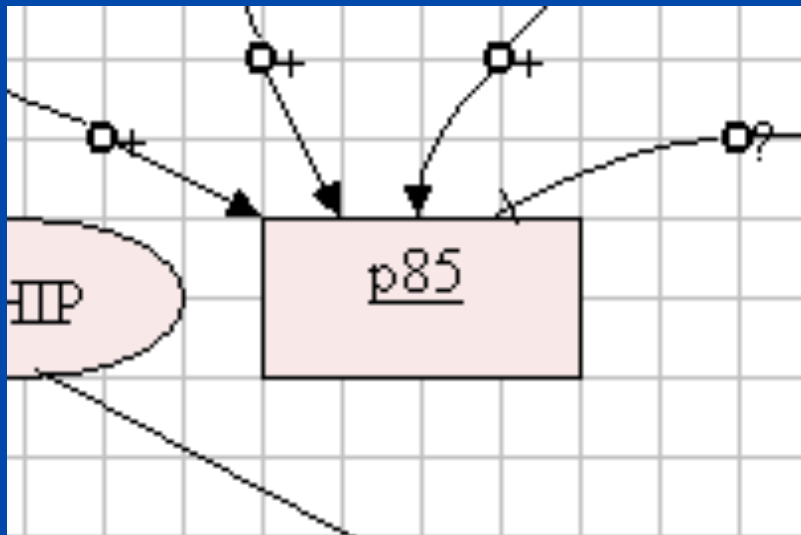
Process

■ *Process* visualizes sequence of events, e.g. a biochemical reaction or protein interaction.

   ■ Chemical reactions,

   ■ protein binding
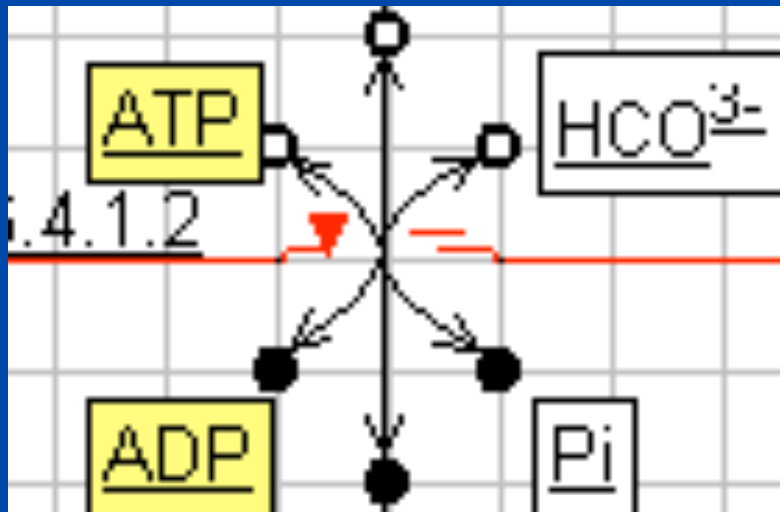
   ■ gene activation

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Link

- *Link* is used to represent any pair-wise relation between objects including "identity" or "act on" relations.

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Label

- *Label* is a visual object to represent textual information and to allow incorporate links to other maps and external resources.

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Types of properties

- Simple data

- Text

- Collections

- Visual data

Simple data

- Simple string of ASCII characters:

  EC: 6.4.1.2

  PubMed: 7567999

Background color	
CID	48
CompoundName	ADP
Foreground color	RGB {0, 0, 0}
Help text	
Hover text	
Line width	2
⊞ Location	[0,60]
Port type	Product
⊞ Size	[8,8]
Stoichiometric coefficient	1
Text	

- Useful for
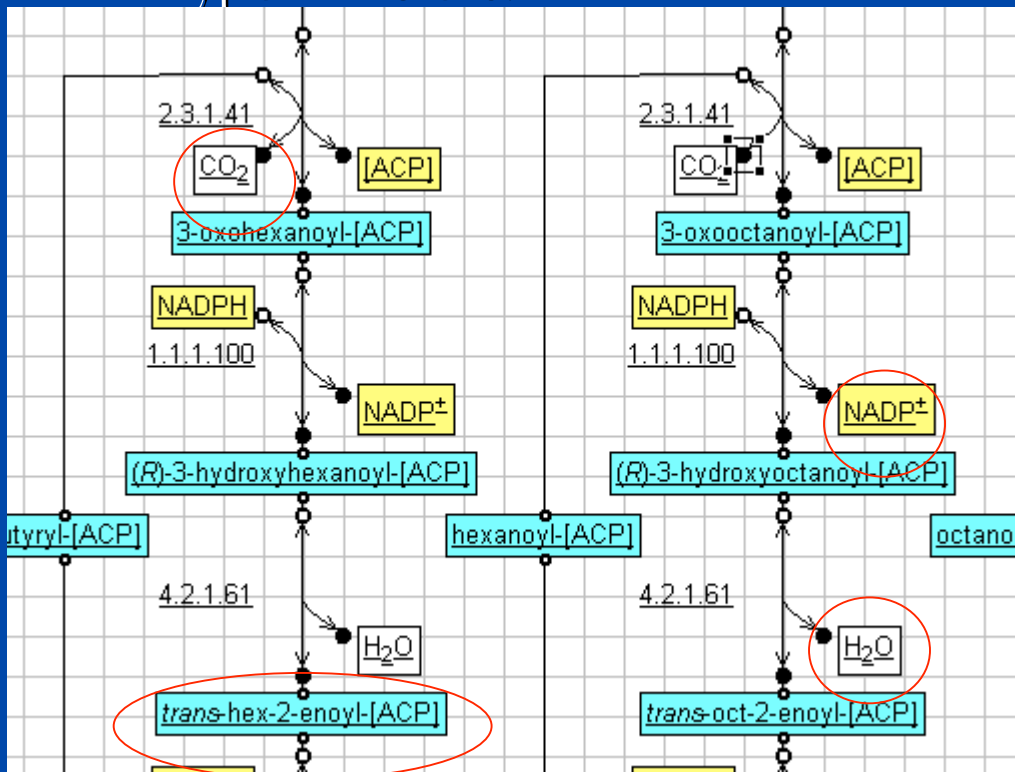 - Internal ID
  - ID in external database (PubMed, GenBank etc.)
  - Abbrevitions
  - Simple descriptions
  - Numerical values (constants, parameters etc.)

Text

- Rich text with formatting, greek letters, fonts, colours, hyperlinks etc.

- Useful for:
  - Name of compounds, proteins etc.
  - Human readable descriptions
  - References to Internet resources
  - References to the other maps

Collections (Text & Simple data)

- List of data of the same type

Background colo	RGB (255, 255, 255)
Foreground colo	RGB (0, 0, 0)
Help text	
Hover text	
Line width	2
⊞ Location	[60,60]
Port type	Source
Shape type	Rectangle
Sites	[text1, text2]
Size	[8,8]
Stoichiometric c	
Text	$Sites$
URL	

- Useful for:
  - List of references (to PubMed)
  - List of synonyms or aliases

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Hyperlinks

- Link the map object with Internet or another map
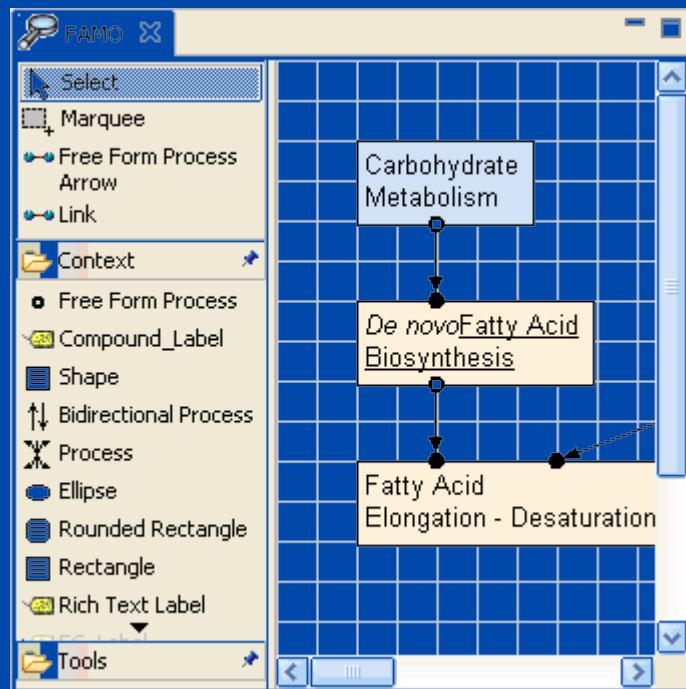
- Useful for:
  - Hierarchical organisation of information
  - Submodels
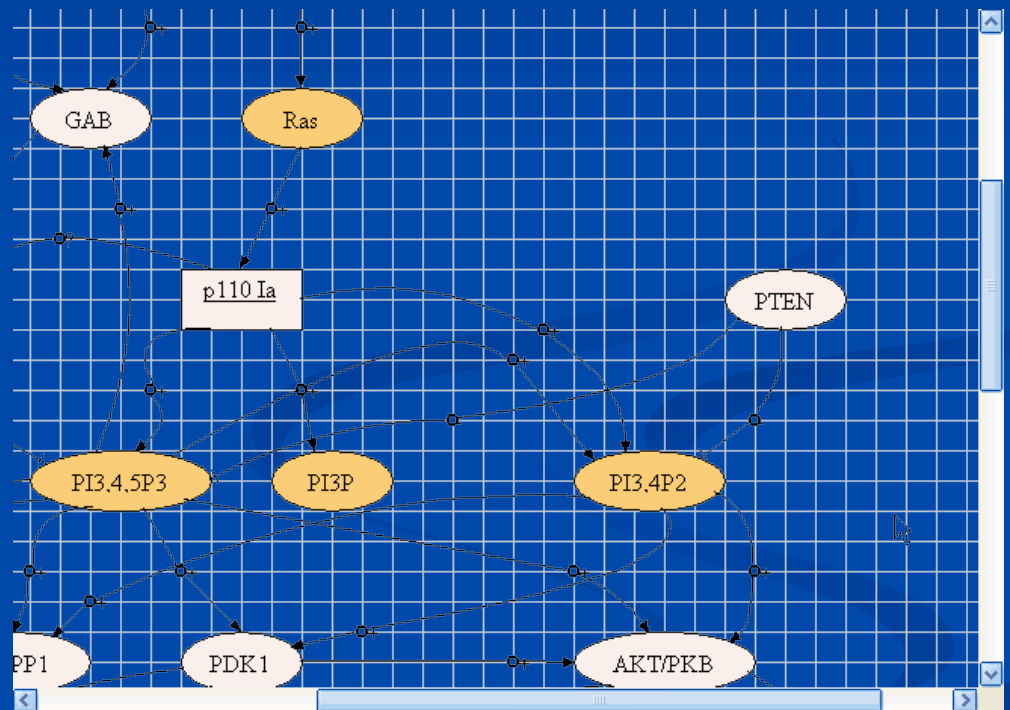 - References to external resources

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Hover text

- Shows text when mouse move over the object
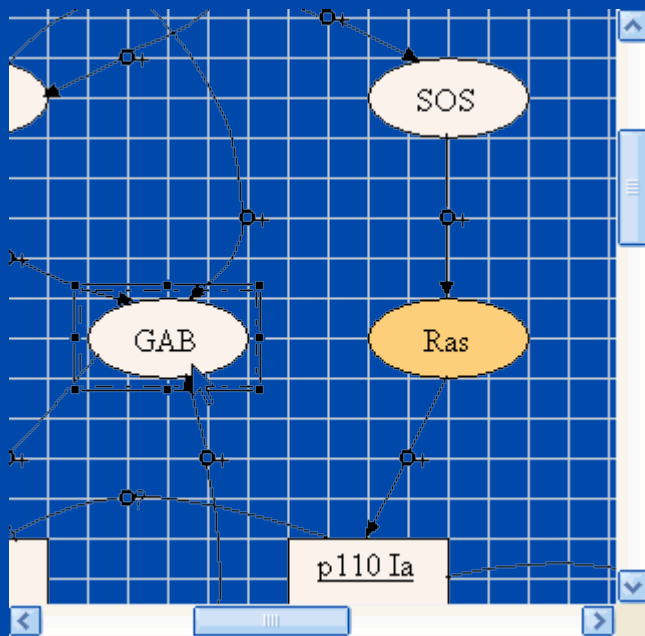
- Useful for
  - Short human readable description of object
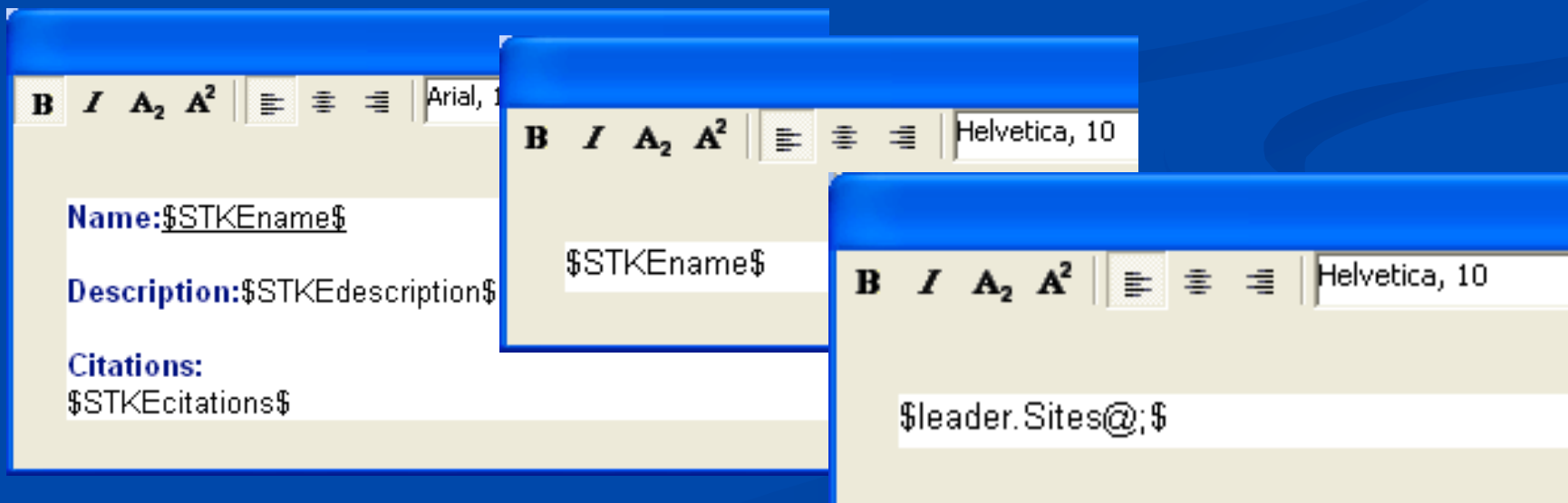 - Summarized view of object properties

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Help text

- Open new pop-up by pressing F2 button
- Useful for:
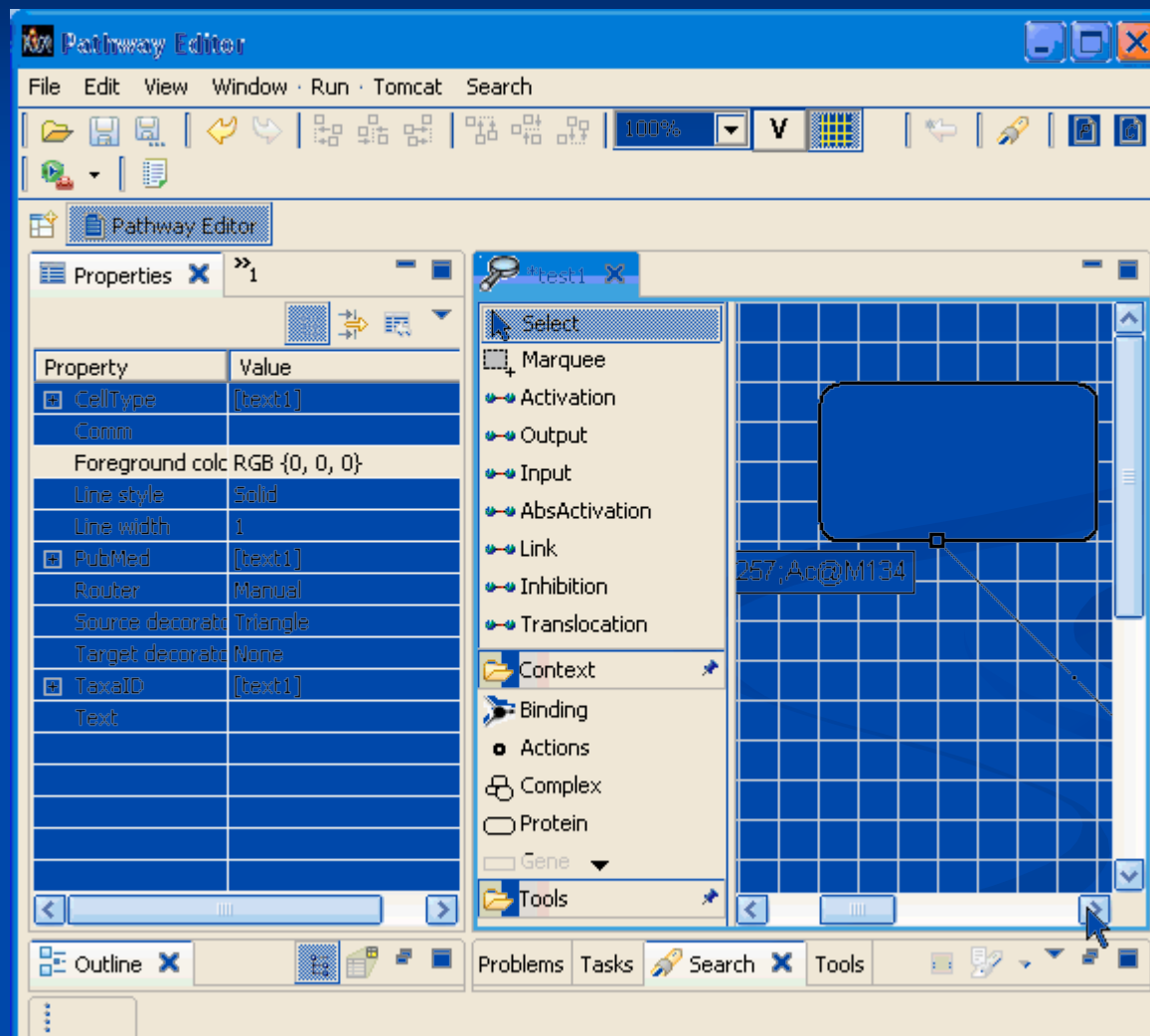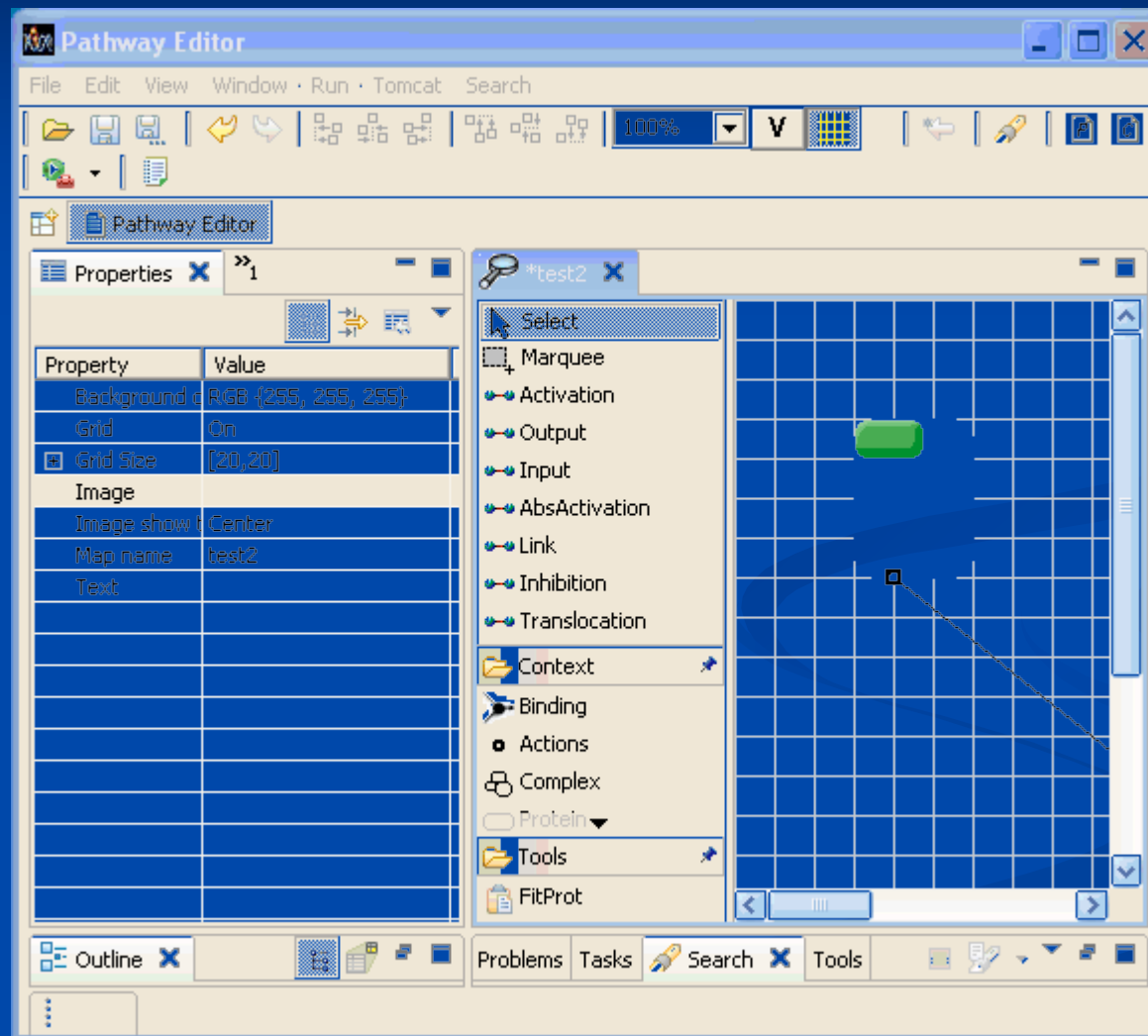 - Extended description of object with hyperlinks etc.

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Reference to value of the property

- There is simple language to reference values of properties of this object or related objects

- Useful for
  - Default values of Help and Hover text
  - Default value of the Label

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Visual properties: colour

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Visual properties: image
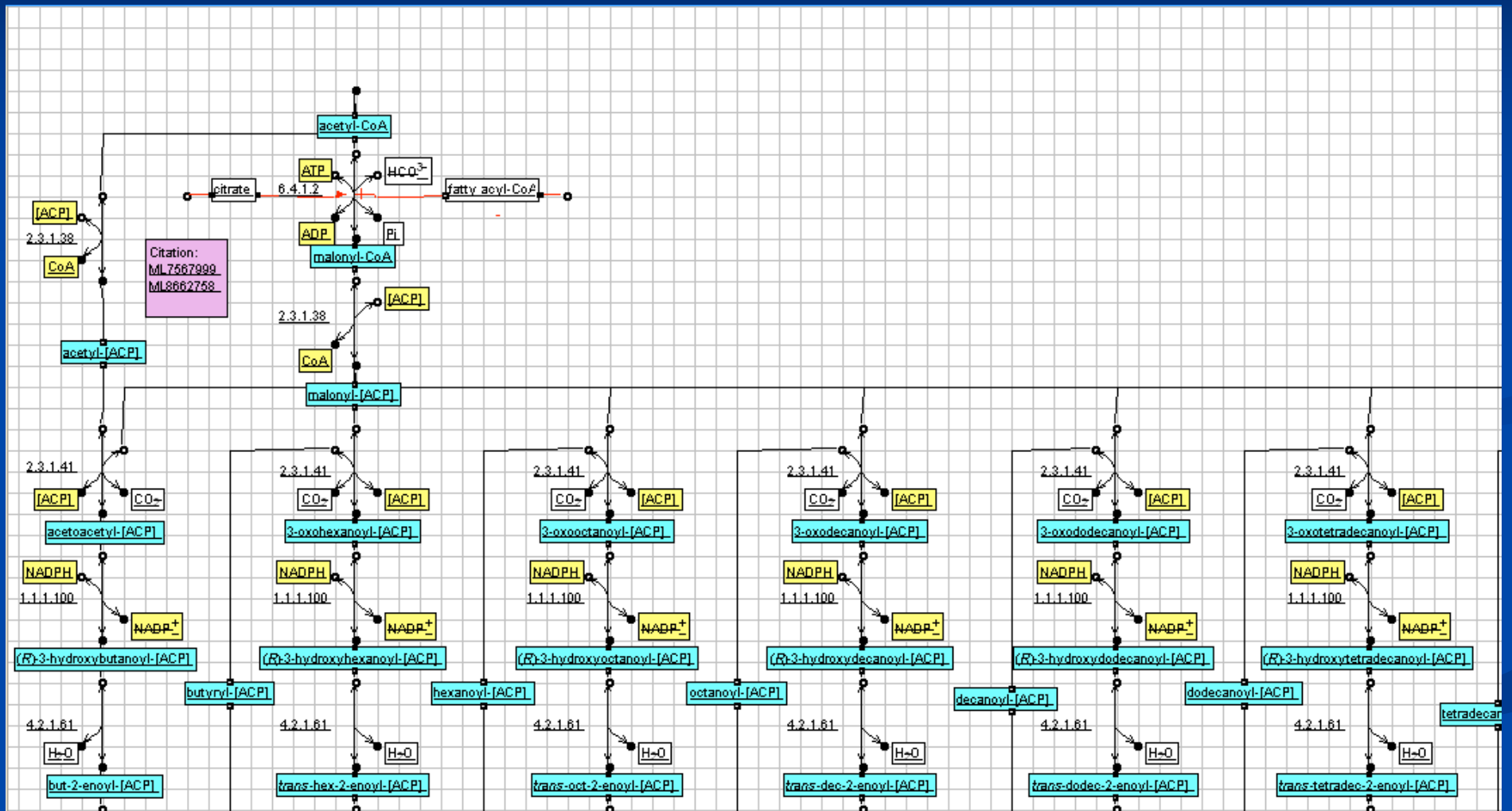
Inheritance, default value

Implemented notations

- EMP/WIT metabolic pathway
- KEGG-like metabolic pathway description
- STKE
- Kitano process notation
- Kitano state notation
- Edinburgh process notation
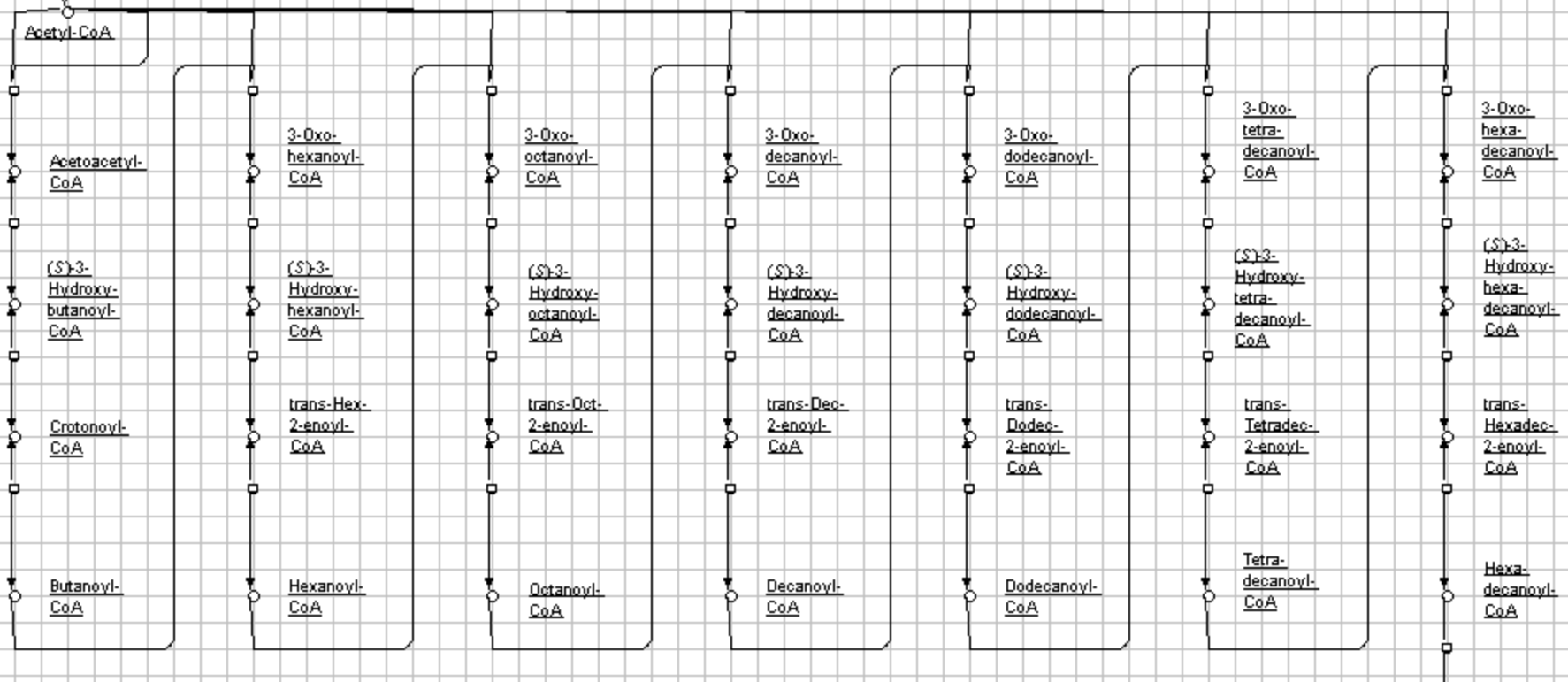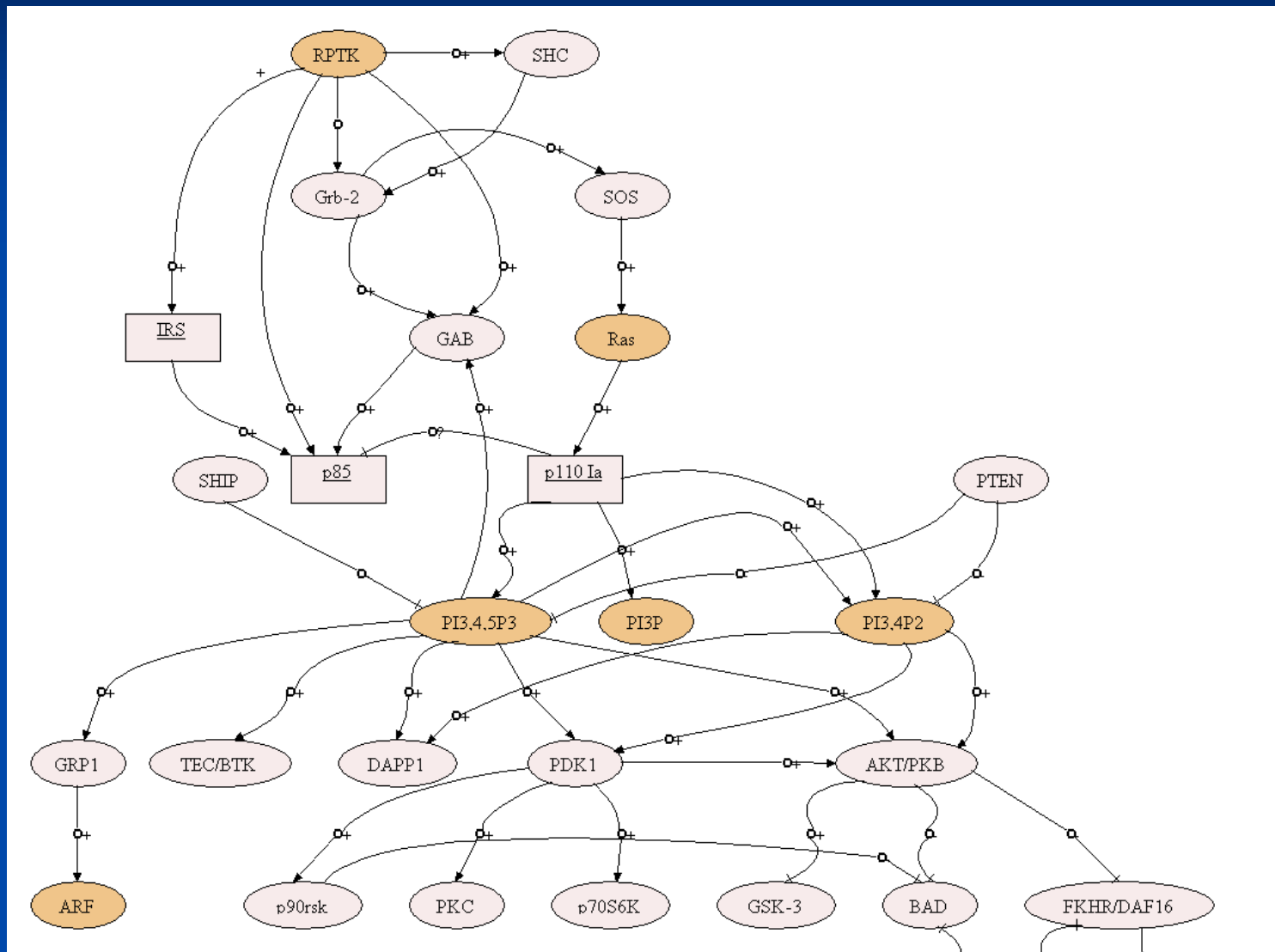- Biocarta-like artistic notation

EMP/WIT outline

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EMP/WIT map

KEGG-like notation

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STKE notation

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Biocarta like noation

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Kitano process notation

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Kitano state notation

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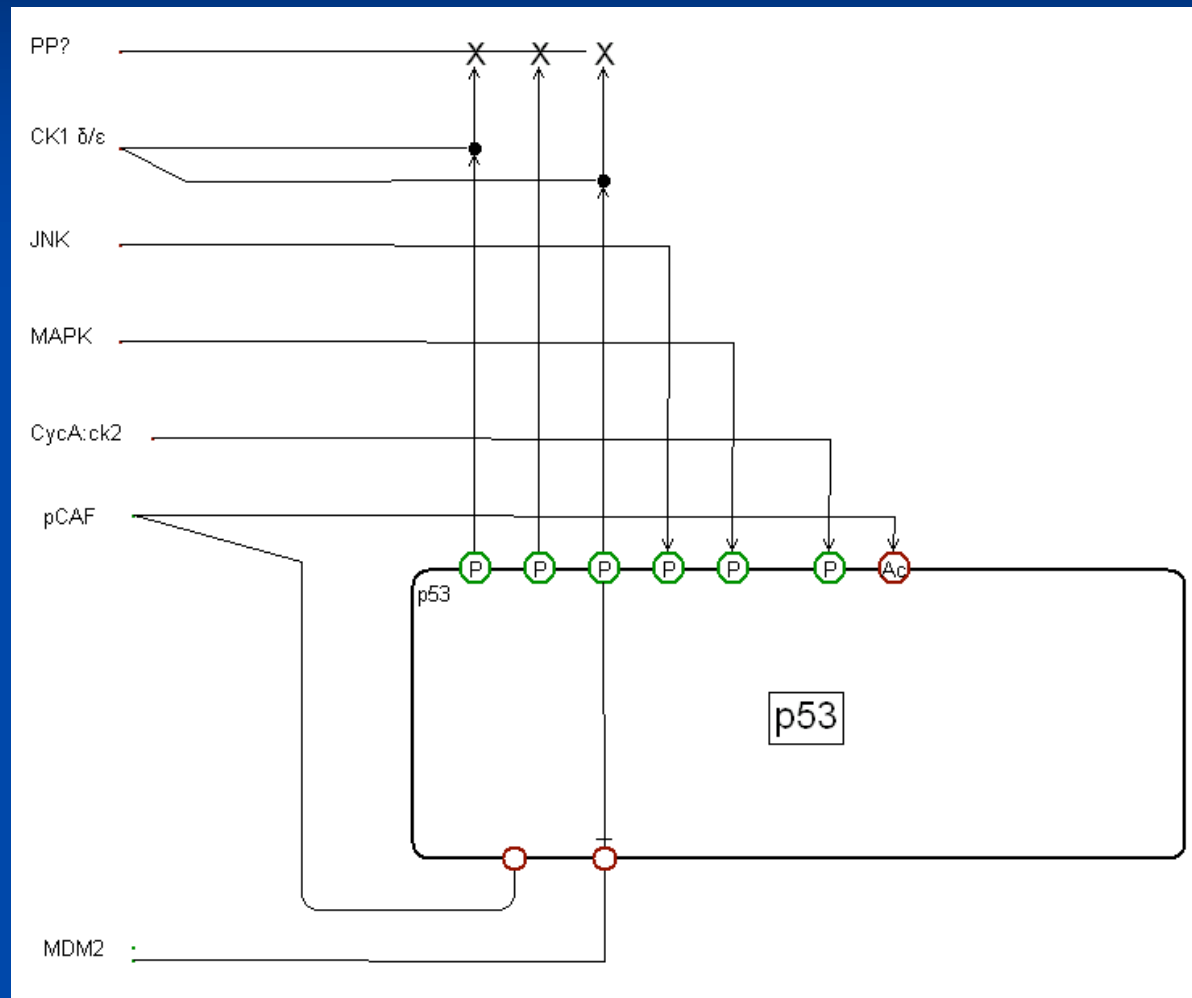
Edinburgh process notation

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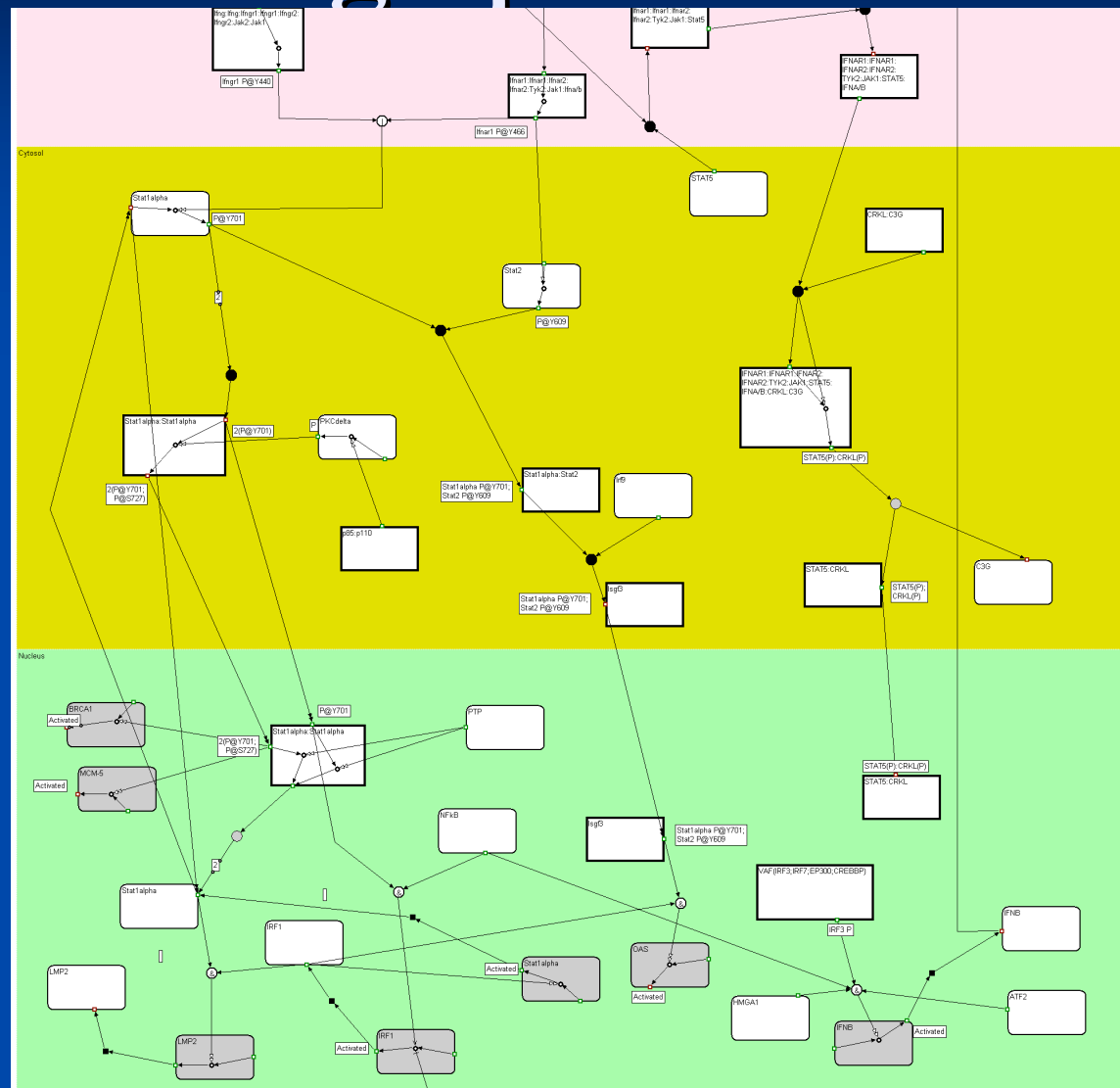
Medium to large model creation

- EPE was used to create
  - Reconstruction of the whole cell *E. coli* metabolism
  - Reconstruction of whole human metabolism
  - Reconstruction of the whole cell *Synechocystis* metabolism
  - Reconstruction of Interferon pathway
  - All KEGG diagrams

System biology modelling gap

"Biologist can be divided into two classes: experimentalists who observed things that cannot be explained, and theoreticians who explain things that cannot be observed."

Katzir-Katchalsky

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Development team

- Kirill Paliy, EMP Project Inc.
- Alex Selkov, EMP Project Inc.
- Serge Dronov, GlaxoSmithKline

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